DEVELOPEMNT OF OPTIMAL MANAGEMENT STRATEGIES FOR CONTAMINATED AQUIFERS INCORPORATING BIODEGRADATION.

A thesis submitted

in the partial fulfillment of the requirements

for the degree of

Master of Technology

by

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to the

DEPARTMENT OF CIVIL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY, KANPUR

DECEMBER, 2004.

CERTIFICATE

This is to certify that the work contained in the thesis entitled "**Development of Optimal Management Strategies for Contaminated Aquifers Incorporating Biodegradation**" by Vudayaraj Sushma has been carried out under my supervision and this work has not been submitted elsewhere for the award of degree.

I.I.T. Kanpur
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ABSTRACT

Groundwater is contaminated by different kind of pollutants and in particular, contamination by organic chemicals is of concern because of the widespread use of these compounds, and because even low concentrations of these chemicals may be very harmful. These contaminants are affected by advection, dispersion, sorption and biological transformations in groundwater systems. However, biological degradation by bacterial populations is the only mechanism where by contaminant mass can be naturally removed from an aquifer. Remediation of a contaminated aquifer can cost hundreds of millions of rupees. Optimization models can be solved for developing optimal cost-effective strategies for remediation of contaminated groundwater aquifers. Incorporation of a numerical simulation model within an optimization model is often very difficult. As an alternative, optimization algorithms are externally linked with groundwater flow and contaminant transport simulation models to determine spatial and temporal management strategies. Especially when the contaminant is an organic chemical like hydrocarbons, it is possible that the remediation may occur through biodegradation in addition to withdrawal from the aquifer. In this study, a Genetic Algorithm based optimization methodology is developed for developing an optimal strategy for control of pollution in an aquifer contaminated by hydrocarbons. The optimization methodology simulates the flow and transport processes in the aquifer through a numerical simulation model externally linked to it, which also incorporates biodegradation. The objective of the developed strategy is to minimize the total amount of pumping over space and time, while ensuring that the pollutant concentration does not exceed specified permissible limits. The constrained non-linear optimization model is converted into unconstrained non-linear optimization model by using the exterior penalty function method, in which penalty terms are added for each constraint. This unconstrained non-linear problem is then optimized by using Genetic Algorithm. The developed methodology is evaluated for an illustrative study area, for different management scenarios, considering Toluene as the organic pollutant. These evaluation results show that the developed methodology is potentially applicable for optimal management of an aquifer contaminated by a biodegradable organic pollutant. Further evaluations are no doubt necessary to establish its applicability to real life aquifer remediation problems.

DEDICATED TO MY PARENTS

ACKNOWLEDGEMENT

I take this opportunity to express my immense gratitude to my thesis supervisor Dr. Bithin Datta who has guided me at all nodes of my thesis with utmost patience and support. It's been an enlightening experience to work under the guidance of my esteemed supervisor. All the discussions that I had with him were enthusiastic and developed independent thinking in me.

I also take this opportunity to express my sincere thanks to Dr. Ashu Jain, Dr. T. Gangadharaih, Dr. Rajesh Srivastava, Dr. Onkar Dikshit, Dr. Kalyanmoy Deb, Dr. Bhaskar Dasgupta who have enriched my knowledge and interest in the courses taught by them. I wish to thank some of the seniors Chandra Rupa, Deepesh Singh, Raj Mohan Singh, Suresh Kartha, and Sampath Kumar for their support.

I wish to thank all my classmates Ajay Das, Anirban Dhar, Antima Jain, Avinash Vasudeo, and Renu Singhal for their support and affection during my entire stay in IITK. I also wish to thank my friends Basha, Bharathi, Gautham, G. Sushma, Krishna, Papa Rao, Rohini, Rupal, Satya, Siva, and Vanitha, for making my stay at IITK the most memorable one. My special thanks go to Anil for his all time assistance through out my thesis. I thank the entire faculty, staff and student community in IIT Kanpur for creating a wonderful environment.

I'm extremely grateful to my entire family for all the support and advice they have given that have finally helped me reach this stage.

Kanpur, India.

December, 2004.

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CONTENTS

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Introduction

Groundwater contamination by organic chemicals is of concern because of the widespread use of these compounds, and because even low concentrations of these chemicals may be very harmful. Dissolved organic contaminants are affected by advection, dispersion, sorption and biological transformations in groundwater systems. However, biological degradation by bacterial populations is the only mechanism where by contaminant mass can be naturally removed from an aquifer. Artificially introduced bacterial population can be also used to clean up aquifers contaminated by various pollutants.

Remediation of a contaminated aquifer can cost hundreds of millions of rupees. Optimization methods can potentially identify solutions that can save significant amounts of money. Optimization models can be solved for developing optimal cost-effective strategies for remediation of contaminated groundwater aquifers. Any such optimization model needs to incorporate the simulation of the physical processes in the aquifer. Incorporation of a numerical simulation model with in an optimization model is often very difficult. As an alternative, optimization algorithms can be combined with groundwater flow and contaminant transport simulation models to determine spatial and temporal management strategies. Also spatial and temporal distribution of pumping can be used to control or remediate a contaminated aquifer. Especially when the contaminant is an organic chemical like hydrocarbons, it is possible that the remediation may occur

through biodegradation in addition to withdrawal from the aquifer. Optimal control applications that are as large-scale as those generally arising in groundwater-remediation problems require special optimization algorithms. These algorithms should be highly efficient numerically, and should be able to deal with nonlinearities that arise.

In this study, a Genetic Algorithm based optimization methodology is developed for developing a strategy for control of pollution in a aquifer contaminated by hydrocarbons. The optimization methodology simulates the flow and transport processes in the aquifer through a numerical simulation model externally linked to it. The biodegradation process due to indigenously present bacterial population is also incorporated in the simulation model. Therefore, the developed optimal management strategy accounts for the biodegradation of the hydrocarbon pollutant. The objective of the developed strategy is to minimize the total amount of pumping over space and time, while ensuring that the pollutant concentration does not exceed specified permissible limits.

The constrained non-linear optimization model is converted into unconstrained non-linear optimization model by using the exterior penalty function method. The exterior penalty function method is a technique for converting a constrained optimization problem into an unconstrained optimization problem by adding penalty terms for each constraint. This unconstrained non-linear problem is then optimized by using Genetic Algorithm. The developed methodology is evaluated for an illustrative study area, for different management scenarios, considering toluene as the organic pollutant.

1.2 Specific Objectives:

The specific objectives of this thesis work are:

1. Implementing a two-dimensional, solute-transport model with biodegradation for an illustrative study area.
2. Development of a linked simulation-optimization methodology for optimal control of biodegradable pollutants in a contaminated aquifer using genetic algorithm and an externally linked numerical simulation model.
3. Evaluating the performance of the developed methodology for an illustrative study area for different management scenarios.

1.3 Literature Review

Development of an optimal strategy for groundwater pollution remediation has become an active area of research in the last several years, because of the high cost of remediation and the potential of optimization methods to reduce the cost substantially. A variety of optimization methods have been utilized, and a number of optimization models have been developed by different researchers. The main objective of this study is to develop an optimization model for optimal control of biodegradable pollutants in a contaminated aquifer. This chapter reviews the published body of work related to the groundwater flow and transport simulation models, linked simulation-optimization models, and the role of Genetic Algorithm (GA) as an optimization tool in the field of groundwater management.

1.3.1 Groundwater Flow and Solute-Transport Simulation

Groundwater solute-transport simulation modeling is an important tool that aids in the analysis of groundwater contamination problems, both actual and potential.

Accidental spills, leakage, and waste disposal operations can lead to ground-water contamination. The ability to analyze and predict the movement of solutes in ground-water systems is necessary to assess the effects of a contamination situation, or properly design a waste-disposal operation. Also, simulation modeling can be used to compare alternative strategies for aquifer reclamation.

The groundwater flow and contamination models are classified according to the characteristics of usage, function and simulation (Reddi et al., 1997).

- Usage – Predictive purposes, Management Purposes or Parameter identification.
- Function – Flow simulation, Contaminant transport or Energy transport.
- Simulation - Domain representation, Dimensionality or Solution technique involved.

There are many groundwater flow simulation models available in literature. Some of them are HELP, DCM3D, ODAST, SOIL, DPCT, MAT123D, RETCF77, UNSAT (-H, -2), GEOFLOW, GW FLOW, MOD3D, PLASM (flow models) and ODAST, DPCT, MAT123D, PORFLO-3D, PORMC-3, TOUGH, RANDOM WALK, CFEST, SOLUTE PKG., VAM2D, 3-D MIXING CELL, FLOWTHROUGH, MOC, SEFTRAN, SWIFT, TARGET, TRACER3CD (flow and transport models) (Reddi et al., 1997).

The environmental fate and transport of a contaminant is controlled by the compound's physical and chemical properties, the properties of the subsurface media and geochemical and biological conditions in the zone through which the compound is migrating. The in situ processes that determine the rate of groundwater contaminant migration and natural attenuation are (source 30):

- Physical: advection, dilution, diffusion, dispersion and volatilization.

- Chemical: chemical (abiotic) degradation reactions, sorption and desorption.
- Biological: aerobic and anaerobic bio-degradation.

The different biodegradation models available in the literature are Bioscreen, Biochlor, BIOPLUME II and III, MT3D, RT3D, MS, SEAM 3D, Bio1D, Bio2D (Minsker and Shoemaker, 1998), and (sources 31, 32), BIOMOC (Essaid and Bekins, 1997).

Borden and Bedient, (1986) developed equations for simulating the simultaneous growth, decay, and transport of micro-organisms, as well as the transport and removal of hydrocarbon and oxygen. These equations were solved by conventional numerical techniques to study the impact of microbial kinetics, horizontal mixing, adsorption and vertical exchange with the unsaturated zone on biodegradation.

Borden et al., (1986) applied the above developed model to an abandoned creosoting site where biodegradation is known to occur. The loss of hydrocarbon due to horizontal mixing with oxygenated ground water and resulting biodegradation is simulated by generating oxygen and hydrocarbon distributions independently and then combining by superposition. This procedure is only applicable where absorption of hydrocarbon is negligible. The major transport parameters were obtained by calibrating the model to a chloride plume also present at the site.

Baveye and Valocchi (1989) derived a mathematical model for the transport of biologically reacting solutes in saturated soils and aquifers, which involves no unwarned assumption for the distribution of the microorganisms in the pore space. Some of the consequences of similarities between microscopic transport equations obtained in

different conceptual frameworks of bacterial growth are discussed from an operational standpoint and in terms of model validation.

Macquarrie et al., (1990) developed a physically and biochemically based numerical solution for the transport of biodegradable organic solutes with emphasis on an efficient numerical approach. A dual-Monod relationship, combined with the advection-dispersion equation, is used to represent the biological and physical processes affecting the organic solute, electron acceptor, and microbial population. The principal direction finite-element technique that is more accurate and efficient than standard finite-element techniques has been successfully applied to the problem of biodegradable organic solute transport.

Chen et al., (1992) developed a one-dimensional numerical model for simulating the biodegradation and transport of benzene and toluene in the subsurface environment. Modeled processes include mass exchange between the constituent phases (solid, liquid, gas, and biomass), advective and dispersive, two electron acceptors, one trace nutrient, and two microbial biomass productions. This work illustrated the utility of a comprehensive experimental/modeling approach for the enhancement of our understanding of biodegradation processes in porous media.

Essaid et al., (1995) developed and tested a two dimensional, multispecies reactive solute transport model with sequential aerobic degradation processes. This computational model is a modified version of the MOC (Konikow and Bredehoeft, 1978) model developed by U. S. G. S. and is called as BIOMOC. BIOMOC(Essaid and Bekins, 1997) allows for the simulation of several simultaneously occurring biodegradation

reactions including multiple substrate uptake, sequential terminal electron acceptor use, and cellular nutrient limitation of biomass growth.

1.3.2 Linked Simulation – Optimization

The use of simulation models to describe the behavior of solutes in groundwater systems has become an important tool in hydrogeologic investigations. Often, solute transport simulation studies are undertaken with the ultimate aim of evaluating aquifer management alternatives. In such situations the need is not for a simulation model alone, but for a combined simulation and optimization based management model. The combined model should contain an accurate representation of the particular system under consideration and should enable optimal management of the aquifer. In recent years several researchers have demonstrated the role of linked simulation-optimization modeling in the aquifer management.

Gorelick and Remson (1982) used a linear solute transport simulation model to generate a unit source-concentration response matrix that was incorporated into a management model. The linear programming-superposition method was implemented for managing multiple sources of groundwater pollution over time. The objective of this study was to optimally manage several groundwater pollutant sources over time so as to maximize disposal potential while meeting distributed groundwater quality constraints.

Gorelick (1982) combined linear programming with U. S. Geological Survey solute transport simulation model MOC (Konikow and Bredehoeft, 1978) to maximize the waste disposal potential while maintaining water quality at several observational wells. The decision variables of the management model were solute waste disposal rates at various facilities distributed over space. A concentration response matrix obtained

from the simulation model was used in the management model to describe transient solute transport. The objective of this study was for simultaneous utilization of an aquifer for waste disposal and for water supply.

Gill et al. (1984) combined finite element groundwater flow and contaminant transport simulation with nonlinear optimization to determine the optimal design of reclamation schemes for contaminated groundwater systems. The simulation model used here is a subset of SUTRA. The model was capable of identifying well locations and determining pumping and recharges rates for optimal (although not necessarily globally optimal) aquifer restoration design.

Chang et al. (1992) developed a management model to compute time-varying pumping rates for remediation of contaminated groundwater by combining a nonlinear, distributed parameter, groundwater flow and contaminant transport simulation model with a constrained optimal control algorithm. Their results showed that time-varying pumping policies can be more economical than time invariant pumping policy for situations in which the plume boundaries move a significant distance relative to the radius of influence of the pumping wells.

Rogers and Dowla (1994) developed an optimization methodology using artificial neural networks (ANNs) with parallel solute transport modeling to optimize aquifer remediation. They simulated the complex groundwater scenarios with a two-dimensional hybrid finite-difference/finite-element flow and transport computer code. The input of the ANN characterizes the different realizations of pumping, with each input indicating the pumping level of a well. The output is capable of characterizing the objectives and constraints of the optimization, such as attainment of regulatory goals, value of cost

functions and cleanup time, and mass of containment removal. The search is directed by a simple genetic algorithm. The results of this study suggest that the ANN approach has more advantages over the conventional technique for the test cases. The performance of the ANN model was tested by varying the problem formulation, network architecture, and learning algorithm.

Ritzel et al. (1994) linked finite difference model MOC (Konikow and Bredehoeft) with GA to solve a multiple objective groundwater pollution containment problem. Their objective was to find a set of optimal solutions on the trade-off curve between reliability and cost of a hydraulic containment system.

Minsker and Shoemaker (1996) developed an optimal control model for improving the design of in situ bioremediation of groundwater. They implemented a finite element biodegradation simulation model, Bio2D and optimal control theory algorithm. The derived analytical derivatives of the bioremediation finite element model are used in the optimal control algorithm.

McKinney and Lin (1996) developed a groundwater management model using a nonlinear programming algorithm to find the minimum cost design of the combined pumping and treatment components of a pump-and-treat remediation system including the fixed costs of system construction and installation, as well as operation and maintenance.

Datta and Dhiman (1996) developed a mathematical model by linking a groundwater pollution transport simulation model and an optimization model for designing an optimal groundwater quality-monitoring network. The model was formulated using chance constraints and was solved by using a mixed integer

programming algorithm. They simulated the transport of radioactive pollutant Tritium, using a finite difference based, two-dimensional numerical model.

Culver et al., (1997) implemented dynamic optimal control algorithm for groundwater remediation to incorporate treatment facility capital costs, as a function of the peak operating rate. This work demonstrates that capital treatment costs may significantly impact a dynamic management policy, and that these capital costs should be explicitly incorporated into a dynamic management model. They demonstrated a straightforward method of incorporating the capital costs of a groundwater treatment system into a dynamic optimal control algorithm.

Culver and Shenk (1998) evaluated the performance of a dynamic optimal control algorithm while utilizing a more accurate description of the costs associated with a granular activated carbon treatment system. For the optimization algorithm, quasi-Newton differential dynamic programming is combined with a simulation model, a modified version of ISOQUAD. This work suggests that improvements in the differential dynamic programming algorithm may be needed for it to be a robust technique for realistic nonconvex objective functions.

Minsker and Shoemaker (1998) developed a methodology for quantifying the uncertainty associated with error in optimal decision models. They developed a decision model by coupling a nonlinear groundwater transport simulation model, Bio2D with an optimization algorithm called successive approximation linear quadratic regulator (SALQR), which is used to determine the most cost-effective well locations and pumping rates for in situ bioremediation.

Yoon and Shoemaker (1999) linked BIO2D, a two dimensional finite-element simulation model with eight optimization algorithms comprising of evolutionary algorithms (binary-coded GA, real-coded GA, and derandomized evolution strategy), direct search methods (Nelder-Mead simplex, modified simplex, and parallel directive search), and derivative based optimization methods (implicit filtering for constrained optimization and successive approximation linear quadratic regulator) to compare their computational performance in identifying the most cost-effective policy for in situ bioremediation of contaminated groundwater.

Hilton and Culver (2000) developed an optimization model by combining GA with a 2D groundwater flow and transport simulation model BIO2D-KE. The developed optimization model was applied to two pump-and-treat design examples, and compared two methods, the additive penalty method (APM) and the multiplicative penalty method (MPM) for constraint handling within the genetic algorithm framework

Chan Hilton and Culver (2001) evaluated the sensitivity of optimal remedial design policies and their associated costs to the residual constraint violation, using a genetic algorithm. The optimization model developed by linking GA to the simulation model BIO2D-KE was applied to solve two different groundwater remediation design problems: pump-and-treat using granular activated carbon and enhanced in situ bioremediation.

Aksoy and Culver (2004) investigated the impacts of physical and chemical aquifer heterogeneities on optimal remediation design, costs, and time to compliance by linking a genetic algorithm with BIO2D-KE, a contaminant transport simulation model.

1.3.3 Genetic Algorithms in Groundwater Management

In the mid-1960's the process of natural evolution intrigued John Holland of the University of Michigan, who developed computational techniques which simulated the evolution process and applied to mathematical programming leading to the evolution of Genetic algorithm (GA). Genetic algorithms provide an alternative to gradient-based techniques for solving complex and highly non-linear optimization problems (McKinney and Lin, 1994). The GA has been used in wide variety of applications in the field of water resources (Ritzel et al., 1994).

Ritzel et al., (1994) investigated the ability of genetic algorithm to solve a multiple objective groundwater pollution containment problem. They described the simple GAs and also GAs that can solve multiple objective problems. Two different GAs, a vector evaluated GA (VEGA), and Pareto GA were formulated. Also found the set of optimal solutions on the trade-off curve between the reliability and cost of a hydraulic containment system. For the zero-fixed cost situation, the Pareto GA was shown to be superior to the VEGA and was shown to produce a trade-off curve similar to that obtained via another optimization technique, mixed integer chance constrained programming (MICCP).

McKinney and Lin (1994) incorporated groundwater simulation models into a genetic algorithm to solve three groundwater management problems: maximum pumping from an aquifer, minimum cost water supply development, and minimum cost aquifer remediation.

Huang and Mayer (1997) developed an optimization model using genetic algorithm for dynamic groundwater remediation management by simultaneously using well locations and the corresponding pumping rates as the decision variables. The well location search path and convergence behavior indicated that the genetic algorithm is an effective alternative solution scheme, and that well location optimization is more important than pumping rate optimization.

Yoon and Shoemaker (1999) compared the computational performance of eight optimization algorithms that are used to identify the most cost-effective policy for in situ bioremediation of contaminated ground water. They concluded that the binary GA is consistently slower and less accurate than all the other algorithms tested.

Hilton and Culver (2000) compared two methods, the additive penalty method (APM) and the multiplicative penalty method (MPM) for constraint handling within the genetic algorithm framework. An optimization model was developed by combining GA with a 2D groundwater flow and transport simulation model BIO2D-KE. The developed model was applied to two pump-and-treat design examples. The results demonstrated that the MPM was a robust method, capable of finding feasible and optimal or near-optimal solutions while using a range of weights.

Chan Hilton and Culver (2001) evaluated the sensitivity of optimal remedial design policies and their associated costs to the residual constraint violation, using a genetic algorithm. The optimization model developed by linking GA to the simulation model BIO2D-KE was applied to solve two different groundwater remediation design problems: pump-and-treat using granular activated carbon and enhanced in situ

Maskey et al., (2002) used four global optimization algorithms, including a popular genetic algorithm to minimize both cleanup time and cleanup cost taking pumping rates and well locations as decision variables. On the basis of the obtained results, Adaptive Cluster Covering (ACCO) was the fastest, but Controlled Random Search (CRS4) and GA were more accurate.

Aksoy and Culver (2004) investigated the impacts of physical and chemical aquifer heterogeneities on optimal remediation design, costs, and time to compliance by linking a genetic algorithm with BIO2D-KE, a contaminant transport simulation model.

As evident from the above review, a number of attempts have been made for developing groundwater remediation strategies using optimization models. More recently, due to its relative simplicity, linked simulation optimization models using genetic algorithms have attracted the attention of researchers. Linking of the numerical simulation model with an optimization model based on classical optimization techniques, especially gradient based techniques had often proved to be too difficult. Linking of the numerical simulation model with a GA based optimization model on the other hand is relatively much simpler and straightforward. In this study, a GA based linked simulation optimization model is developed which aims at minimizing the total withdrawal from an aquifer, while controlling the pollutant concentrations within permissible limits. The biodegradation processes is also incorporated.

Chapter 2

Methodology

2.1 Introduction:

The main objective of this study is to develop and evaluate an optimization model for optimal control of biodegradable pollutants in a contaminated aquifer. The optimization methodology is based on Genetic Algorithm and utilizes an externally linked solute-transport simulation model with biodegradation.

2.2 Simulation Model

There are many well documented, verified and accepted computer models for simulating the flow or transport processes in groundwater (Reddi et al., 1997). These simulation models in general, numerically solve the flow and transport equations to simulate the physical processes in the aquifer. Groundwater simulation models are sometimes also used to evolve management strategies. To do so, a user usually assumes several groundwater pumping strategies (a strategy is a set of pumping schedules and locations). Then the simulation model is used to predict the real-world consequences of implementing each of these strategies and selects the most desirable strategy from among those tested. Because, there are generally an infinite number of strategies possible for a situation, it is less probable that the best possible strategy is identified. Groundwater solute-transport simulation modeling is an important tool that aids in the analysis of groundwater contamination problems, both actual and potential. Accidental spills, leakage, and waste disposal operations can lead to groundwater contamination. The ability to analyze and predict the movement of solutes in groundwater systems is

necessary to assess the extent and effects of a contamination. Simulation modeling is also used sometimes to compare alternative strategies for aquifer reclamation.

The equations that describe the groundwater flow and transport processes may be solved using different types of models. Some models may involve exact solutions to equations that describe very simple flow or transport conditions (analytical model) and others may involve approximations of equations that describe very complex conditions (numerical models). Each model may also simulate one or more of the processes that govern groundwater flow or contaminant migration rather than all of the flow and transport processes. In selecting a model for use at a site, it is necessary to determine whether the model equations account for the key processes occurring at the site. Each model, whether it is a simple analytical model or a complex numerical model, may have applicability and usefulness in hydrogeological and remedial investigations.

In this study, the aim is to evolve an aquifer management strategy using hydraulic (pumping/recharge) controls, for a biodegradable hydrocarbon pollutant. Therefore, it was essential to choose a simulation model with capability of incorporating biodegradation process. Therefore, the numerical simulation model BIOMOC developed by USGS (Essaid and Bekins, 1997) was chosen for this study. It's a general and flexible two-dimensional transport and biodegradation model that can handle multiple substrates and microbial populations, sequential terminal electron acceptor use and cellular nutrient limitation. BIOMOC is chosen in this study for the following reasons:

- It is two dimensional and applicable to transient condition.
- It can handle single as well as multiple substrates and microbial populations.

- The biomass growth is modeled with specified yield and decay values.
- The rate of the degradation reactions can be represented by single-substrate Monod, multiple Monod, or minimum Monod kinetics.
- Availability of source code.

The simulation model is based on the solution of finite difference forms of the flow and transport equations, which are solved by using the method of characteristics, and particle tracking method, (Essaid and Bekins, 1997). The following discussion of the BIOMOC model is based on Essaid and Bekins (1997).

- **Flow Equation:**

$$S\frac{\partial h}{\partial t}=\frac{\partial}{\partial x_j}\left(bK_{jk}\frac{\partial h}{\partial x_k}\right)-W \qquad \text{j, k} = 1, 2 \qquad (1)$$

Where S is the storage coefficient, h is the hydraulic head (L), t is time (T), K_{jk} is the hydraulic conductivity tensor (LT^{-1}), b is the aquifer thickness (L), W is the source fluid flux (positive for outflow and negative for inflow) expressed as volumetric flux per unit area (LT^{-1}), and x_j and x_k are Cartesian coordinates (L).

By Darcy's Law, the average linear flow velocity in the x_j direction (V_j) is given by

$$V_j=-\frac{K_{jk}}{\varepsilon}\frac{\partial h}{\partial x_j} \qquad (2)$$

Where ε is the effective porosity (dimensionless).

- **Transport Equation**

$$R_i\frac{\partial C_i}{\partial t}=\frac{1}{b}\frac{\partial}{\partial x_j}(bD_{jk}\frac{\partial C_i}{\partial xk})-V_j\frac{\partial}{\partial x_j}C_i+\frac{W(C_i-C_i')}{(\varepsilon b)}-R_i\lambda_i C_i-B_i \qquad (3)$$

j,k =1,2

Where C_i is the concentration of the i^{th} solute (ML^{-3}), R_i is the retardation factor for the i^{th} solute, D_{jk} is the dispersion tensor (L^2T^{-1}), C_i' is the concentration of the i^{th} solute in the source fluid (ML^{-3}), λ_i is the first order decay rate constant (T^{-1}) for the i^{th} solute (half life $t_{1/2} = (\ln 2)/\lambda$, and B_i is the biodegradation reaction rate term ($ML^{-3}T^{-1}$) representing the total uptake of the i^{th} solute due to all active biodegradation processes.

- **Biodegradation Terms**

The total uptake of any solute i is given by the summation of the uptake for all simultaneously occurring biodegradation processes.

$$B_i = \sum_{n=1}^{N} \beta_i^n v^n \tag{4}$$

Where N is the total number of biodegradation processes, v^n is the uptake rate of substrate by biodegradation process n ($ML^{-3}T^{-1}$), and β_i^n is the uptake coefficient of solute i for biodegradation process n.

In this methodology, multiple Monod formulation is used to represent the growth and substrate uptake rate, which assumes that the biodegradation reaction is limited by the concentration of each of the substances involved in the reaction (Essaid and Bekins, 1997).

$$v^n = \frac{V^n{}_{\max}}{I_{nc}} \left\{ \left(\frac{C_1}{K^n{}_1 / I_c + C_1 + I_h} \right) \left(\frac{C_2}{K^n{}_2 / I_c + C_2 + I_h} \right) \cdots \left(\frac{C_m}{K^n{}_m / I_c + C_m + I_h} \right) \right\} \frac{X^n{}_k}{I_b} \tag{5}$$

Where V^n_{max} is the asymptotic maximum specific uptake rate of the substrate (T^{-1}), and K_n is the half-saturation constant (ML^{-3}). X^n_k is the biomass concentration of microbial population k responsible for biodegradation process n (ML^{-3}). I_{nc}, I_c, and I_b are the noncompetitive, competitive, and biomass inhibition factors respectively, given by I=1 +

Q_s/k_s where Q_s is the concentration of the inhibiting substance s (ML^{-3}) and k_s is the inhibition constant for that substance (ML^{-3}).

The biomass inhibition factor for microbial population, k, is given by

$$I_b = 1+X_k/k_{biok} \tag{6}$$

Where k_{biok} represents the biomass concentration above which the growth of population k becomes limited. I_h represents inhibition cost by the presence of compounds that are toxic where

$$I_h = \sum C^2{}_{ii} / k_{hii} \tag{7}$$

is the sum of overall inhibiting compounds each with concentration C_{ii} and k_{hii} is the Haldane inhibition constant for each *ii* compound.

2.3 Genetic Algorithm (GA) Based Optimization:

Optimization models have proved to be a powerful and useful method to solve design and operation problems associated with groundwater hydraulic control, water supply, and remediation. A suitable nonlinear optimization technique is required to solve the formulated optimization model. Genetic Algorithm is chosen to solve the single-objective optimization model, as GA is especially suitable for solving linked simulation-optimization models.

Genetic Algorithms are a family of combinatorial optimization methods that search for solutions of complex problems using an analogy between optimization and natural selection. These algorithms were developed by Holland and coworkers at the University of Michigan. GA provides an alternative to gradient-based techniques for solving complex and highly non-linear optimization problems (McKinney and Lin, 1994).

2.3.1 Working Principle of GA:

GAs use a random search procedure inspired by biological evolution, cross-breeding trial designs and allowing only in the *fittest* designs to survive and propagate to successive *generations*. To solve an optimization problem, GA encodes the decision variable values as *substrings* of binary digits. These substrings of decision variables are concatenated to from longer strings or *chromosomes* representing a solution to the problem. The entire *population* of such designs represents a *generation*. The GA searches for an optimal design by comparing the fitness of the independent population. A population of such strings is generated and each member string is assigned an objective function or *fitness* value based on how well the design performs. The fitness values of members of the population are compared with each other and the fittest members are more likely to undergo *reproduction* and propagate to the next generation. The reproduction process is controlled by *crossover* and *mutation*. The population of designs is allowed to evolve through successive generations until a termination criterion is met (McKinney and Lin, 1994).

2.3.1.1 Encoding and Decoding

A binary coded GA is used in this study. Binary coded GA encodes each decision variable as a binary substring of a particular length according to the precision required. For understanding the decoding process, the decoding of the decision variable, pumping rate $P_i = \{P_1, P_2, \ldots\ldots P_k\}$ is explained. The variable P_i has a string length of l_i, defined in the limits of $[P_{min}, P_{max}]$. The decoding function is

$$P_i = P_{min} + \frac{P_{max} - P_{min}}{2^{l_i} - 1} \sum_{j=0}^{l_i} b_j 2^j \tag{8}$$

From the above decoding function, the precision value of the variable attained is $\frac{(P_{max} - P_{min})}{(2^{l_i} - 1)}$. Knowing the desired precision and lower and upper bounds of each variable, a lower bound of the string size required to code the variable can be obtained.

After a population of strings is initialized, a series of three genetic operators are applied to the population: (1) Selection, (2) Crossover, and (3) Mutation.

2.3.1.2 Selection:

To select which strings in the population get to reproduce, the *fitness* of each string must be determined. The decoded decision variables are used to determine the value of the objective function. The objective function value is usually used to represent the string's fitness. The fittest strings from the population are the selected to reproduce. There are many selection methods used available in the literature ranking selection, tournament selection etc. The selection method used in this study is stochastic remainder roulette wheel selection (Deb, 2002).

2.3.1.3 Crossover:

The crossover operator is used to create new solutions from the selected individuals. This operator exchanges the gene information between solutions in the mating pool, after the crossover site of the selected strings. The genetic operation of crossover is performed on each mated pair with a certain probability, referred to as a crossover probability. The crossover probability parameter is typically set so that crossover is performed on most, but not all, of the population (Ritzel et al., 1994).

2.3.1.4 Mutation:

Mutation is performed by altering the value of the selected gene, 0 to 1 or vice versa, in order to maintain the diversity of the population and to prevent GA from

prematurely converging onto a local optimum. This process is controlled by mutation probability (Ritzel et al., 1994).

2.3.1.5 Termination Criteria:

The drawback of most evolutionary optimization techniques including genetic algorithm is that a solution is *better* only in comparison to other, presently known solutions. It has no concept of an *optimal solution*, or any way to test whether a solution is optimal. (For this reason, genetic algorithms are best employed on problems where it is difficult or impossible to test for optimality.) This also means that a genetic algorithm never knows for certain when to stop, aside from the length of time, or the number of iterations or candidate solutions, that you wish to allow it to explore.

In this study the termination criteria utilized is the number of generations limited by the maximum number of generations specified. The maximum number of generations was specified based on some comparison of the average fitness of the population with the maximum fitness obtained for few preliminary solutions.

Therefore, the termination criteria may be subjective in many cases. Possible termination criteria may include:

- Maximum number of generations.
- No improvement in objective or fitness functions over a specified number of generations.
- Convergence of average population fitness to the maximum fitness obtained.

2.3.1.6 Constraint Handling

In constrained optimization, the satisfaction and violation of the constraints play a vital role in determination of the optimal solution. Any violation of the constraint implies an infeasible solution. Penalty function method is often used to convert a constrained

optimization model to an unconstrained optimization model. In this method, if a constraint is violated at any point, the objective function is penalized by an amount depending on the extent of constraint violation. Penalty terms vary in the way the penalty is assigned. A penalty term is added to the objective function to penalize any infeasible solution. In this study exterior penalty method is adopted, due to the fact that initial feasible solutions need not be specified when using the exterior penalty function method (Deb, 2002).

2.4 Development of Management Methodology

A simulation-optimization model is designed to compute the best management strategy directly. This differs from the function of a simulation model. To use a simulation-optimization model, the model defines the management goal(s) and restrictions on acceptable physical system responses. The simulation-optimization model directly calculates the best groundwater management strategy for the management scenario. The simulation or optimization model does this by coupling mathematical optimization methods with standard simulation models.

The primary objective of this study is to develop single objective optimization based model for the optimal control of biodegradable pollutants in a contaminated aquifer using linked simulation-optimization. As it is difficult to induce a simulation model into the optimization model, external linking is done. The optimization model uses the simulation results from the externally linked simulation model to obtain optimal solutions and hence the optimal management strategies.

2.4.1 The Management Model

The objective of the management model developed in this study is to minimize the summation of pumping rates over space and time for the study area, subjected to the constraint of maintaining the concentration of the pollutant below the permissible limit over space and time. The decision variables of the management model are the pumping rates over space and time, and the concentrations of the pollutants over space and time in the aquifer. The space and time are discretized in terms of spatial grids and time periods. The mathematical representation of the developed model is as follows:

Objective:

$$\text{Minimize} \quad \sum_{t=1}^{n} \sum_{i,\, j \in I} P_{i,j}^{t} \tag{9}$$

Where I denotes the set of specified potential pumping locations (i, j), and n denotes the total number of pumping periods considered.

Subjected to the constraints:

1. The concentration ($C_{i,j}^{t}$) of the pollutant at the end of the pumping period at specified nodes of the study area should be less than or equal to the specified maximum permissible concentration ($C^{*}_{i,j}$) of that pollutant at that location.

$$C_{i,j}^{t} \le C_{i,j}^{*} \qquad \forall (i,j) \quad \forall t \tag{10}$$

2. Specified upper and lower bounds on pumping rates at each specified location at different time periods.

$$P_{i,j}^{t} \ge (P_{i,j}^{t})_{L} \qquad \forall (i,j) \quad \forall t \tag{11}$$

$$P_{i,j}^{t} \leq (P_{i,j}^{t})_U \qquad \forall(i,j) \quad \forall t \tag{12}$$

Where $(P_{i,j}^{t})_L$ is the lower bound and $(P_{i,j}^{t})_U$ is the upper bound specified for pumping at location i,j and time period t.

3. The flow and transport simulation model represent binding constraints of the optimization model, and are satisfied by solving the externally linked numerical simulation model.

$$C_{ij}^{t} = f(b,q,p) \qquad \forall(i,j) \quad \forall t \tag{13}$$

Where, b represents the boundary conditions, q represents the parameter values and p represent the set of pumping values, and f(b,q,p) represents the flow and transport simulation model.

2.4.2 Steps in the Developed Methodology

The simulation model used in this study is BIOMOC, a solute transport model with biodegradation. The GA based optimization algorithm first generates the initial population of pumping rate values, using a random number generator. Each set of the generated pumping rate values are sent to the simulation model which has been implemented for the study area. The simulation is then solved to obtain the resulting concentrations at all nodes of the study area. The concentration values are utilized by the GA based model to compute the corresponding fitness function values for each member of the population. The fitness function is a function of specified objective function and constraint violation.

In the next generation a new population is selected by crossover and mutation, from the members of the population in the earlier generation. Fitness function values for the new population are obtained. This procedure is repeated till the termination criterion

is satisfied. The solution obtained is considered as the optimal management strategy for the aquifer. A flow chart describing the steps involved in the externally linked simulation-optimization model in the present study is shown in figure 2.1. The application of this developed methodology for an illustrative study area, and performance evaluation results are discussed in the next chapter.

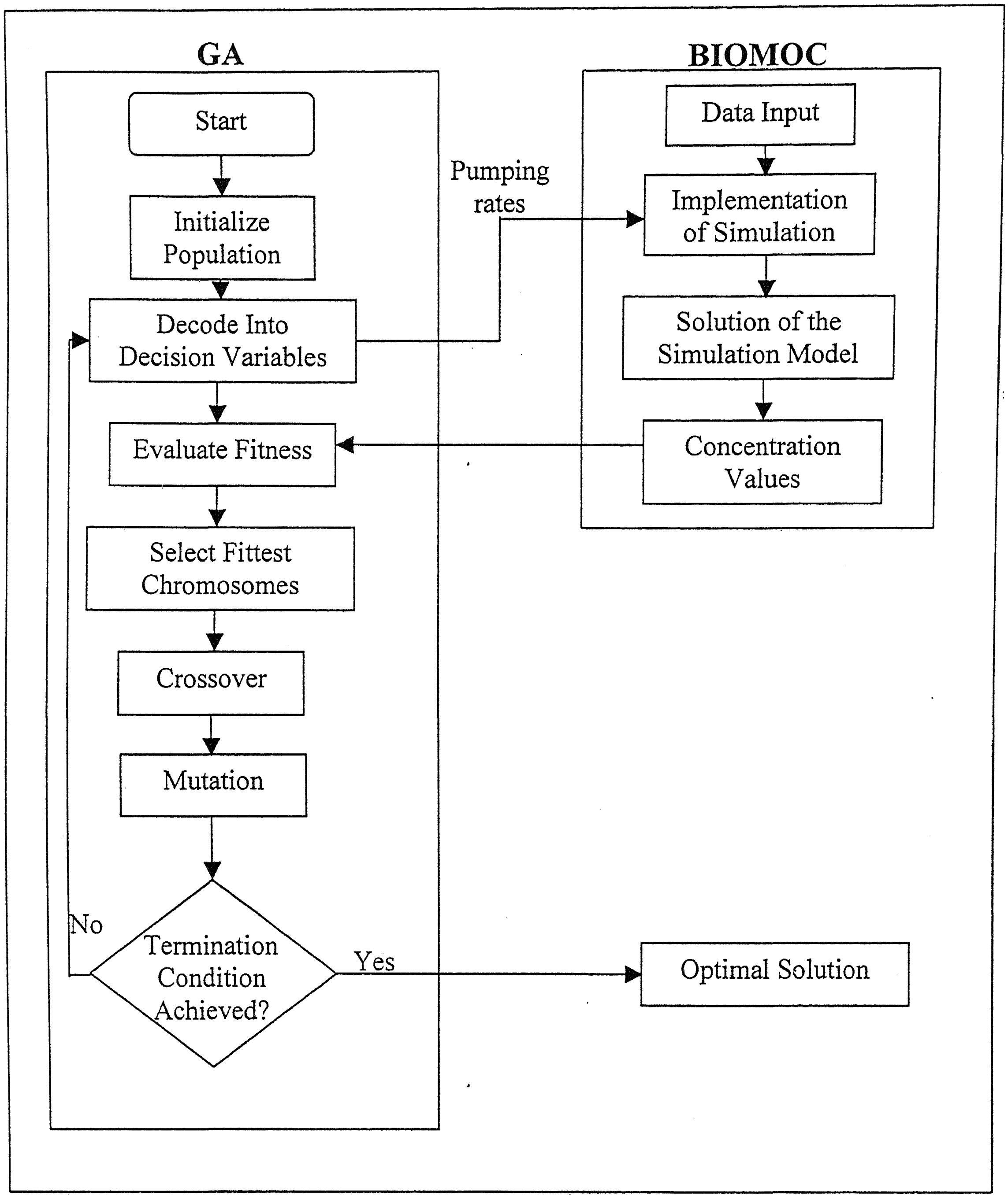


Figure 2.1 Flowchart of Developed Methodology

Chapter 3

Results and Discussions

3.1 Introduction

The formulation of the developed optimization model is presented in chapter 2. The optimization model is externally linked to the simulation model BIOMOC. The solution to this optimization model describes the optimal pumping strategy for the illustrated study area for specified initial and boundary conditions, and hydraulic and biodegradation parameters.

3.2 Study Area

The performance of the model is evaluated by applying the model to an illustrative study area. The study area is assumed as a homogeneous, isotropic, confined aquifer with the dimensions of 1.8 km by 1.3 km in plan and with a uniform thickness of 30.5 m. This study area is discretized by finite difference grids as shown in the figure 3.1. A slight variation of this study area with a modified set of pumping locations is also considered for performance evaluation of the model. Other modified study area is shown in figure 3.2. All other conditions and parameter values are identical for study areas represented by figure 3.1 and figure 3.2.

3.3 Data

The input data required for the simulation model comprises of the aquifer's hydraulic parameters, boundary conditions, the location of wells, their injection and pumping rates, and the biodegradation parameters. The hydraulic and biodegradation parameter values are obtained from Chen et al (1992).

3.4 Assumptions

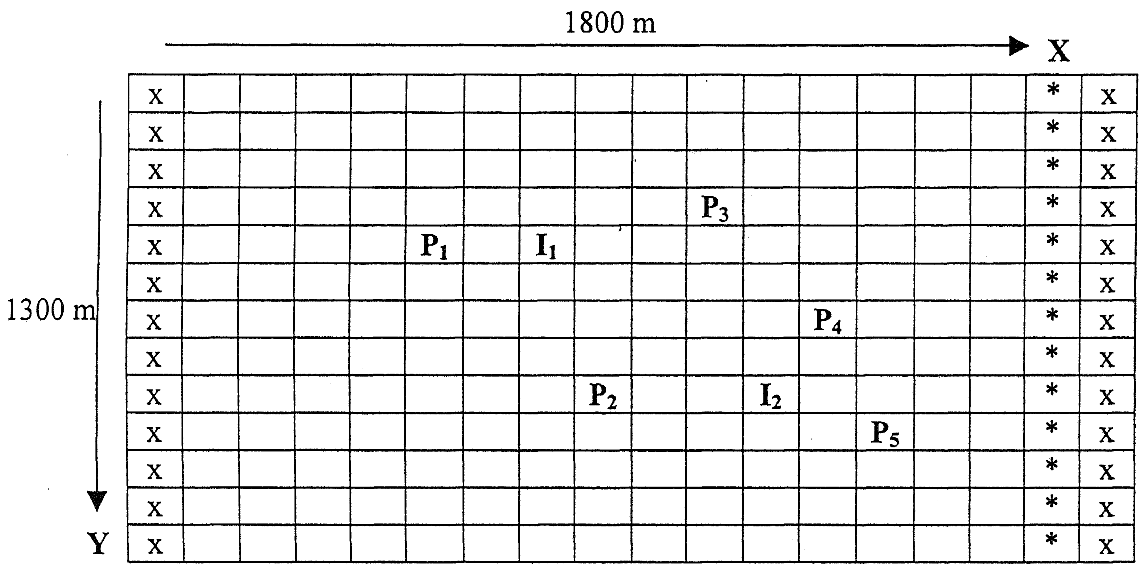
Assumptions made in the development of the simulation model BIOMOC, (Essaid and Bekins, 1997) are also valid here:

1. Flow is two-dimensional.
2. Darcy's law is valid.
3. Porosity and hydraulic conductivity are constant with time, and porosity is uniform in space.
4. Gradients of fluid density, viscosity, and temperature don't affect the velocity distribution.
5. Fluid and aquifer properties are not affected by the reactions that occur.
6. Ionic and molecular diffusion are neglected.
7. The aquifer is homogeneous and isotropic with respect to longitudinal and transverse dispersivity
8. Both the dissolved and sorbed solute phases undergo first order decay. Only the dissolved solute undergoes biodegradation.
9. There is no microbial transport, and the biomass concentration does not drop below the specified initial concentration.
10. A macroscopic approach has been used to represent biodegradation. Biophase diffusion is neglected.

3.5 Model Implementation for the Study Area

The model grid specification is important, as the simulation model needs the finite difference representation of the study area. The study area is represented by 18 x 13 finite difference cells. Each finite-difference cell is 100 m x 100 m, as shown in figure 3.1 and

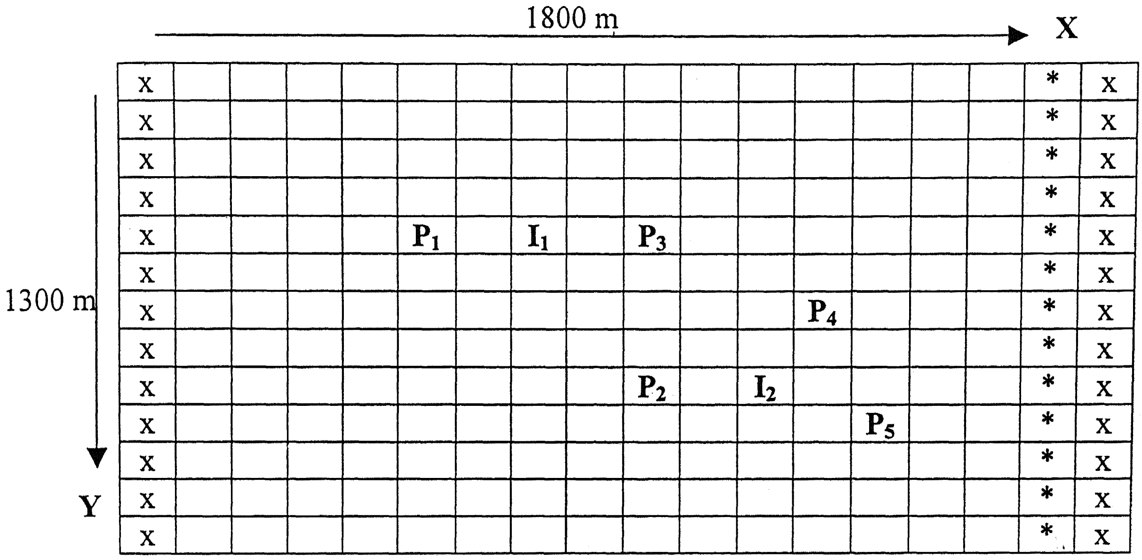
figure 3.2. A constant head (36.59 m) boundary condition is imposed at the left hand side boundary, and a constant head of 26.52m is imposed at the right hand side boundary. The fluid source concentration at these boundary cells is specified as 100 mg/l. the layer of cells just beside (left hand side) the right hand side boundary cells are also specified as constant head cells with zero concentration of the fluid source. The hydraulic head at the intermediate cells is computed by linear interpolation of the hydraulic heads between the right and left hand side boundaries.



x Constant head cells with fluid source concentration of 100 mg/l.

* Constant head cells with zero fluid source concentration.

Figure 3.1. The study area, pumping locations-I



Constant head cells with fluid source concentration of 100 mg/l.

Constant head cells with zero fluid source concentration.

Figure 3.2. The study area, pumping locations-II

The initial values of solute concentration at the internal cells of the aquifer are specified as zero. Two contaminant injection sites are specified at locations I_1 (8,5) and I_2 (12,9) with injection rates of 1 l/s and 1.5 l/s and concentration of 9000 mg/l respectively. The potential pumping locations as specified were varied in this study for evaluation of the solution results. The pumping locations-I are shown in figure 3.1, as P_1 (6,5), P_2 (9,9), P_3 (11,4), P_4 (13,7), P_5 (14,10). The other specified potential pumping locations are shown in figure 3.2 also, as P_1 (6,5), P_2 (10,9), P_3 (10,5), P_4 (13,7), P_5 (14,10). Three management periods each of duration one year are considered in these evaluations. In the present study the pumping rates were assumed same for all the three time periods, as a simplification. Also, the permissible upper limit on pollutant concentration was assumed to be

independent of location and time. The following specifications are made for the management model, as given in table 3.1.

Table 3.1 Management Data

Parameters	Values
Number of pumping periods	3
Number of pumping wells	5
Length of pumping period in years	1

The hydraulic input parameters for the present study are obtained from Chen et al. (1992), as shown in table 3.2.

Table 3.2 Hydraulic Parameters

Parameters	Values
Effective Porosity	0.3
Longitudinal dispersivity	40 m
Storage Coefficient	0.008
Ratio of transverse to longitudinal dispersivity	0.1
Hydraulic Conductivity	1.05×10^{-4} m/s

In the present study, transport and biodegradation of the hydrocarbon pollutant Toluene is simulated for a confined aquifer under transient flow and transport condition. It is assumed that the solute species Toluene follows the multiple Monod kinetics. The mobile particle set representing the solute is assumed to undergo linear sorption, and no decay. The physiochemical parameters used in the simulation model are shown in table 3.3, and are obtained from Chen et al (1992).

Table 3.3 Physiochemical Parameters

Parameters	Values
Linear sorption distribution coefficient of Toluene	0.139 cm^3/g
Soil bulk density	1.67 g cm^{-3}
Decay half life in seconds (no decay)	0

The initial concentration of solute in the aquifer is considered as zero. In this evaluation, only one biodegradation process is simulated and the parameters of the process (Chen et al., 1992) are tabulated in table 3.4.

Table 3.4 Biodegradation Parameters

Parameters	Values
Number of solutes undergoing microbial uptake in the process	1
Asymptotic maximum specific uptake rate V_{max} of the process	1.146 e-04 /sec
Index of microbe population performing the process	1
Yield of the process	0.5
Half saturation constant of toluene	17.4
Uptake coefficient of the toluene	2.19
Death rate of each microbe population	1.157e-06 /sec
Biomass concentration for microbe population	0.82 mg/l

The different parameters of the GA based optimization model are given in table 3.5.Table

Table 3.5 GA Parameters

Parameters	Values
Population size	10
Number of decision variables	701 (pumping and concentration)
Crossover rate	0.8
Mutation rate	0.01
Selection scheme	Stochastic remainder roulette wheel selection
String size per variable	10
Penalty parameter	100.0

The GA optimization algorithm is based on the binary coded, FORTRAN based computer code available at KANGAL library, I.I.T. Kanpur (Deb, 2002).

3.6 Results

The performance evaluation of the proposed methodology was carried out for different scenarios based on the variations of pumping locations, upper limit of pumping, maximum permissible concentration of the solute in the aquifer C^*, and maximum

number of generations specified for the termination of the GA algorithm in the developed linked simulation-optimization model. These, numerical experiments were conducted to verify or intuitively justify the obtained solution results.

To evaluate if there is any improvement in the obtained solution with increase in the maximum permissible number of generations in the GA algorithm, each scenario is run for two different maximum permissible number of generations 100 and 150, each represented as sub scenarios A and B respectively.

The different scenarios considered are shown in table 3.6:

Table 3.6 Scenarios

Scenario	Pumping Location	Upper Pumping Limit of P_1, P_2 l/s	C^* mg/l	No. of Generations
I-A	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	15	10	100
I-B	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	15	10	150
II-A	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	21	10	100
II-B	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	21	10	150
III-A	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	21	5	100
III-B	**P_1(6,5),P_2(9,9),P_3(11,4),P_4(13,7),P_5(14,10)**	21	5	150
IV-A	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	15	10	100
IV-B	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	15	10	150
V-A	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	15	5	100
V-B	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	15	5	150
VI-A	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	21	10	100
VI-B	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	21	10	150
VII-A	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	21	5	100
VII-B	**P_1(6,5),P_2(10,9),P_3(10,5),P_4(13,7),P_5(14,10)**	21	5	150

The different scenarios involved in the present study are explained as follows.

Scenario: I

The maximum permissible concentration, C^* of the solute considered in this scenario is 10 mg/l and the upper limit of pumping is 15 l/s at the pumping wells P_1 (6,5),

P_2 (9,9), P_3 (11,4), P_4 (13,7), P_5 (14,10) in which P_1 and P_2 are located upstream of the injection wells I_1 (8,5) and I_2 (12,9), respectively, as shown in figure 3.1.

Scenario: II

The maximum permissible concentration, C^* of the solute considered in this scenario is 10 mg/l, and the upper limit of pumping is 21 l/s at the pumping wells P_1 (6,5), P_2 (9,9) which are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure 3.1. The upper limit of pumping in wells P_3 (11,4), P_4 (13,7), and P_5 (14,10) is 15 l/s.

Scenario: III

The maximum permissible concentration, C^* of the solute considered in this scenario is 5 mg/l and the upper limit of pumping is 21 l/s at the pumping wells P_1(6,5), P_2 (9,9) which are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure.3.1. The upper limit of pumping for the wells P_3 (11,4), P_4 (13,7), P_5 (14,10) is 15 l/s.

Scenario: IV

The maximum permissible concentration of the solute considered in this scenario is 10 mg/l, and the upper limit of pumping is 15 l/s at the pumping wells P_1 (6,5), P_2 (10,9), P_3 (10,5), P_4 (13,7), P_5 (14,10), in which P_1 and P_2 are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure 3.2. The locations of the pumping wells P_2 and P_3 are shifted nearer to the injection wells compared to the previous scenarios I, II, and III.

Scenario: V

The maximum permissible concentration (C^*) of the solute considered in this scenario is 5 mg/l and the upper limit of pumping is 15 l/s at the pumping wells P_1 (6,5), P_2 (10,9), P_3 (10,5), P_4 (13,7), P_5 (14,10), in which P_1 and P_2 are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure 3.2. The locations of the pumping wells P_2 and P_3 are shifted nearer to the injection wells compared to the previous scenarios I, II, and III.

Scenario: VI

The maximum permissible concentration (C^*) of the solute considered in this scenario is 10 mg/l and the upper limit of pumping is 21 l/s at the pumping wells P_1 (6,5), P_2 (10,9) which are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure 3.2. The upper limit of pumping for the wells P_3 (10,5), P_4 (13,7), P_5 (14,10) is 15 l/s. The locations of the pumping wells P_2 and P_3 are shifted nearer to the injection wells compared to the previous scenarios I, II, and III.

Scenario: VII

The maximum permissible concentration (C^*) of the solute considered in this scenario is 5 mg/l and the upper limit of pumping is 21 l/s at the pumping wells P_1 (6,5), P_2 (10,9) which are on the upstream side of the injection wells I_1 (8,5) and I_2 (12,9) respectively, as shown in figure 3.2. The upper limit of pumping for the wells P_3 (10,5), P_4 (13,7), P_5 (14,10) is 15 l/s. The locations of the pumping wells P_2 and P_3 are shifted nearer to the injection wells compared to the previous scenarios I, II, and III.

The behavior of the fitness function along the generations is as shown in the figures 3.3 to 3.16 for the scenarios I to VII respectively. Solution results were obtained for each of these scenarios, for maximum specified number of generations equal to 100 and 150. These results are presented in the form of plots of fitness function value versus number of generations in figures 3.3 to 3.16. The permissible number of generations was used as a stopping criterion, and these numbers are based on preliminary evaluation of fitness values as a function of the number of generations.

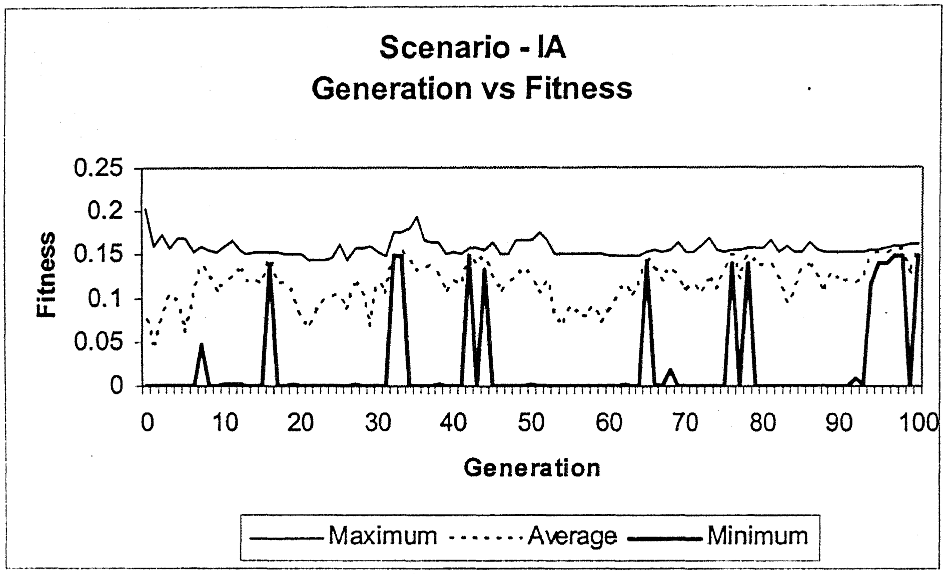


Figure 3.3 Generation vs. Fitness (Scenario-IA).

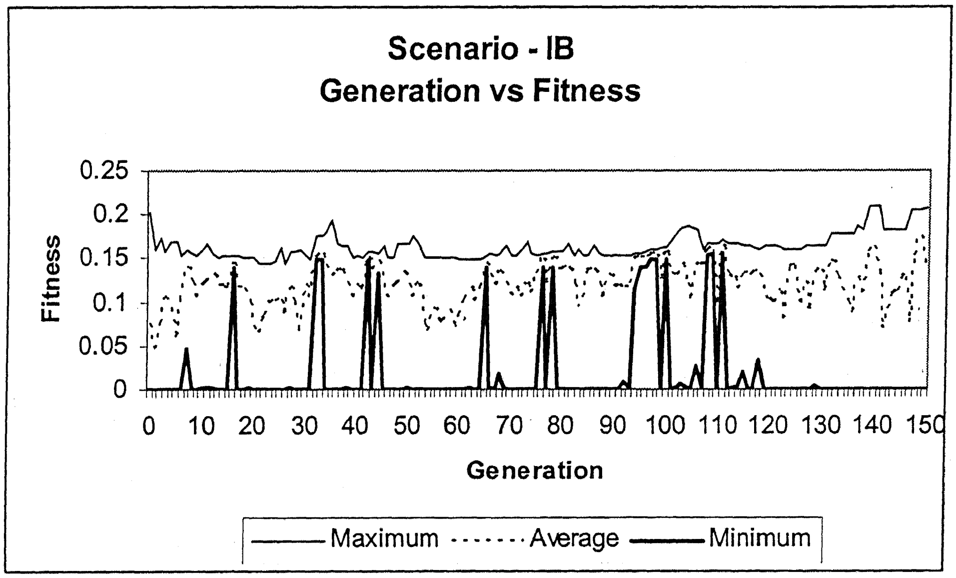


Figure 3.4 Generation vs. Fitness (Scenario-IB).

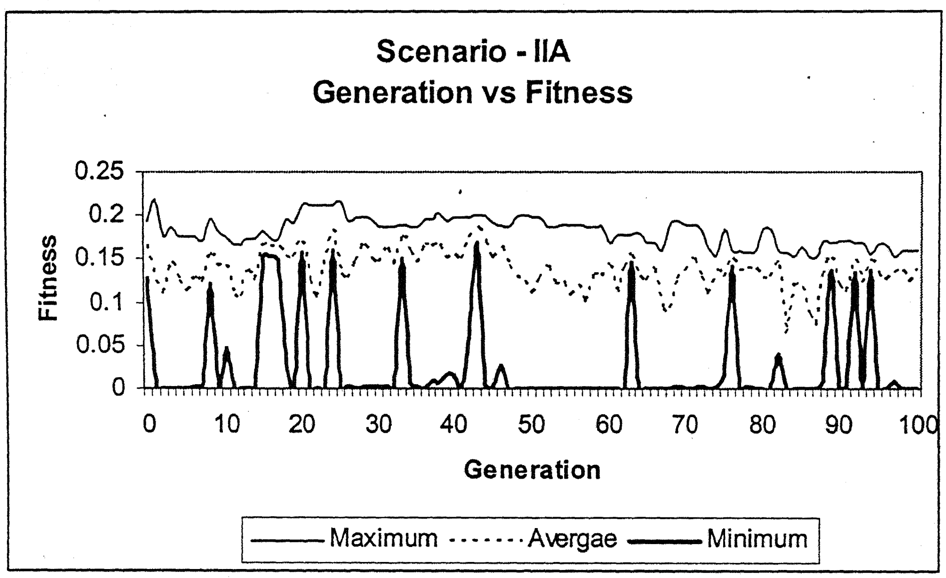


Figure 3.5 Generation vs. Fitness (Scenario-IIA).

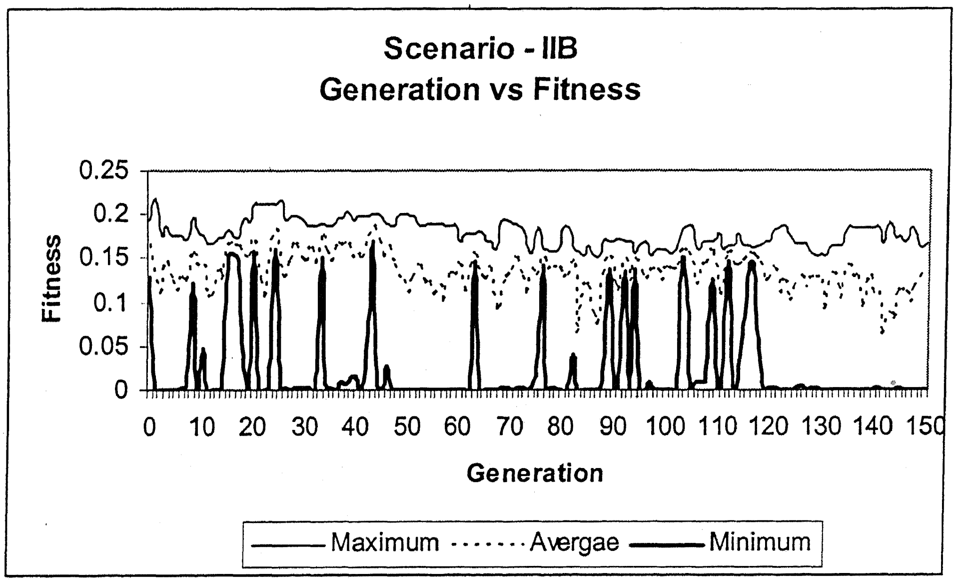


Figure 3.6 Generation vs. Fitness (Scenario-IIB).

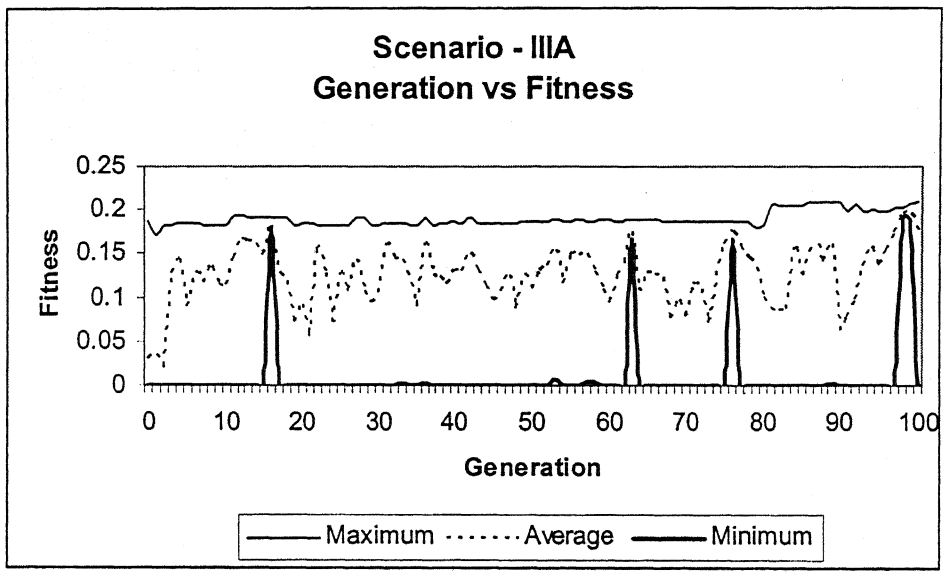


Figure 3.7 Generation vs. Fitness (Scenario-IIIA).

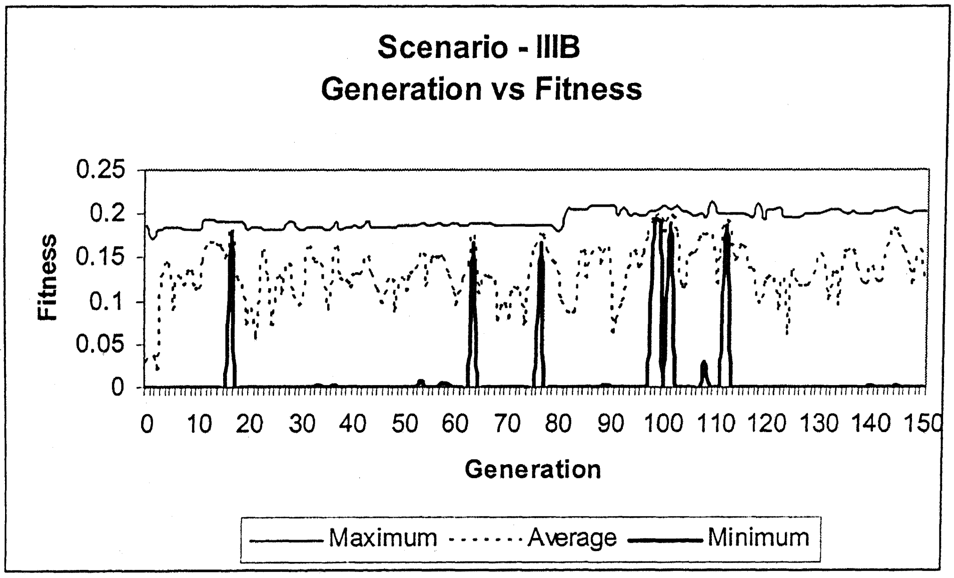


Figure 3.8 Generation vs. Fitness (Scenario-IIIB).

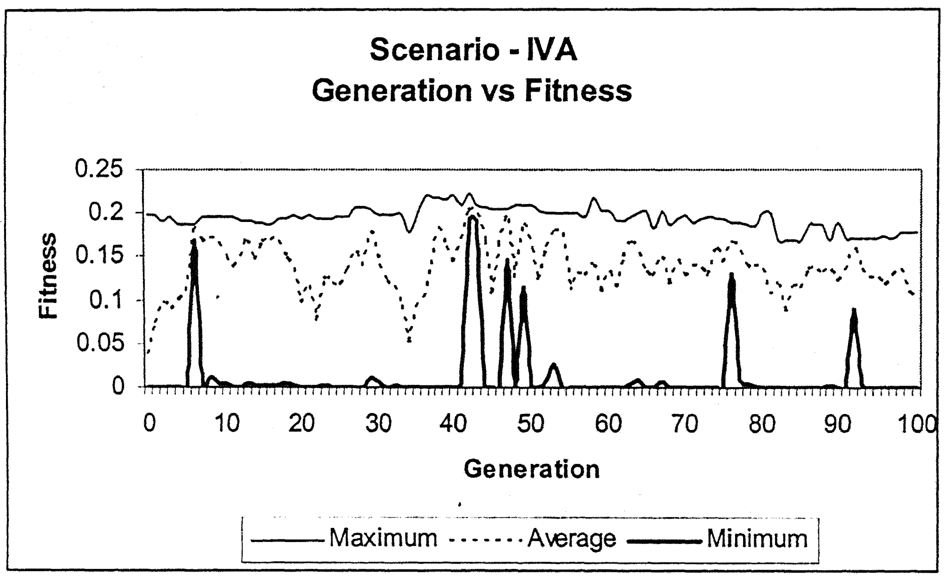


Figure 3.9 Generation vs. Fitness (Scenario-IVA).

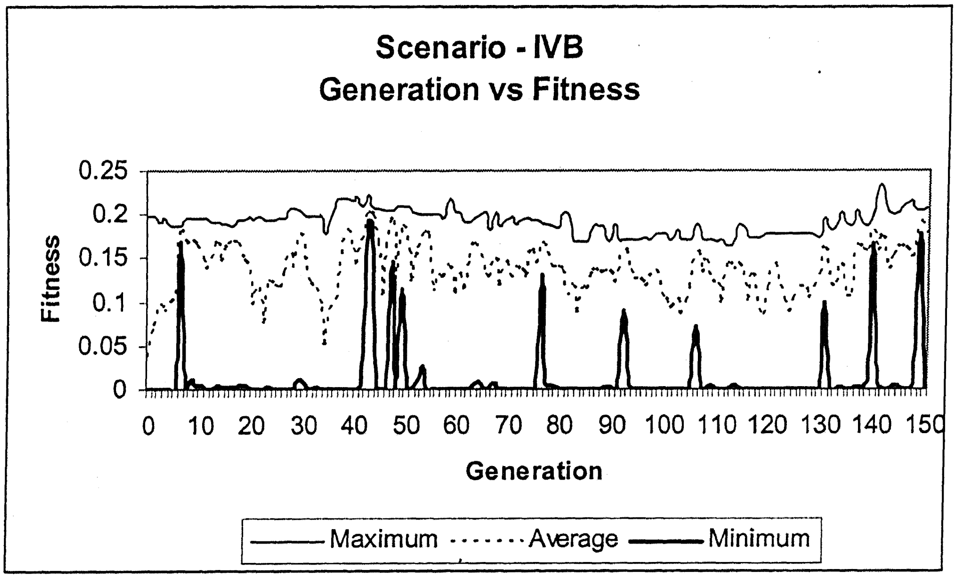


Figure 3.10 Generation vs. Fitness (Scenario-IVB).

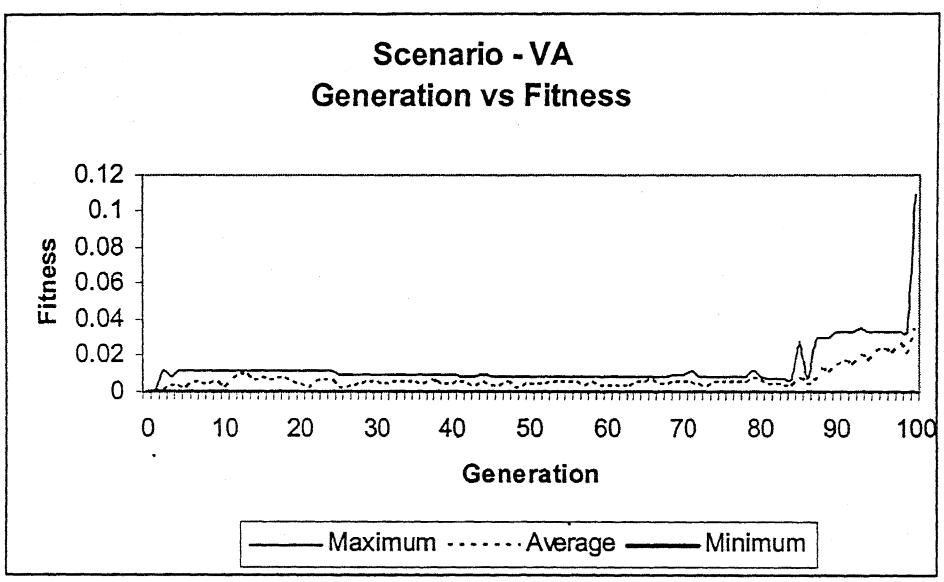


Figure 3.11 Generation vs. Fitness (Scenario-VA).

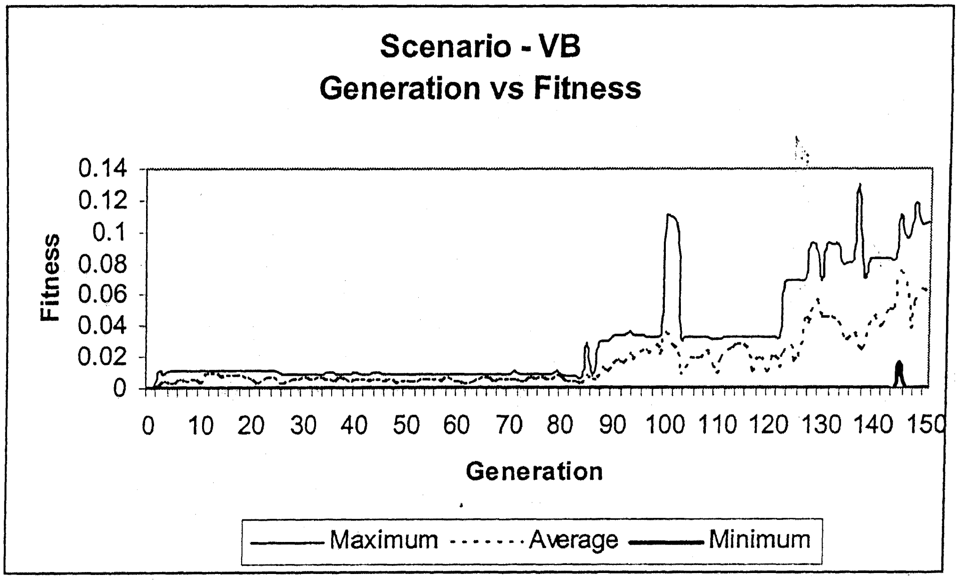


Figure 3.12 Generation vs. Fitness (Scenario-VB).

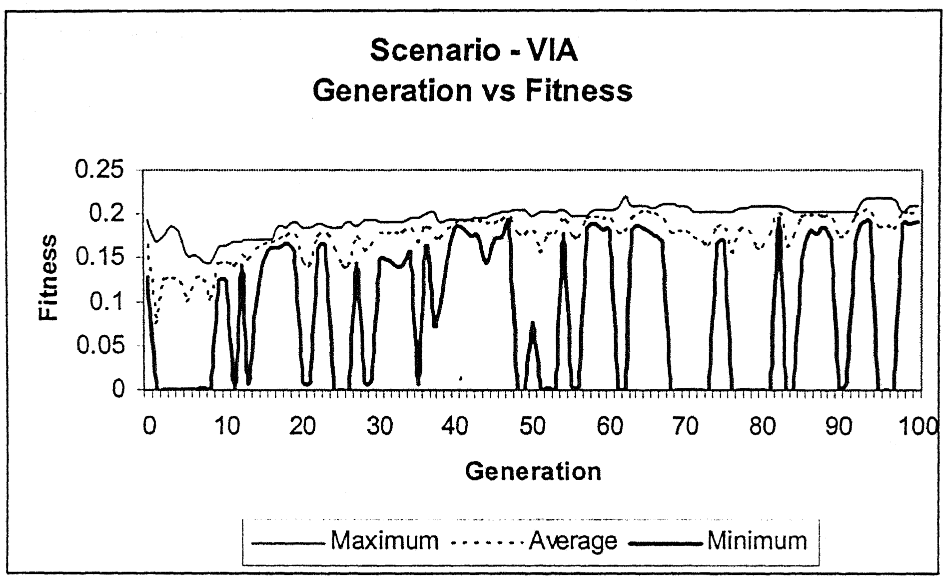


Figure 3.13 Generation vs. Fitness (Scenario-VIA).

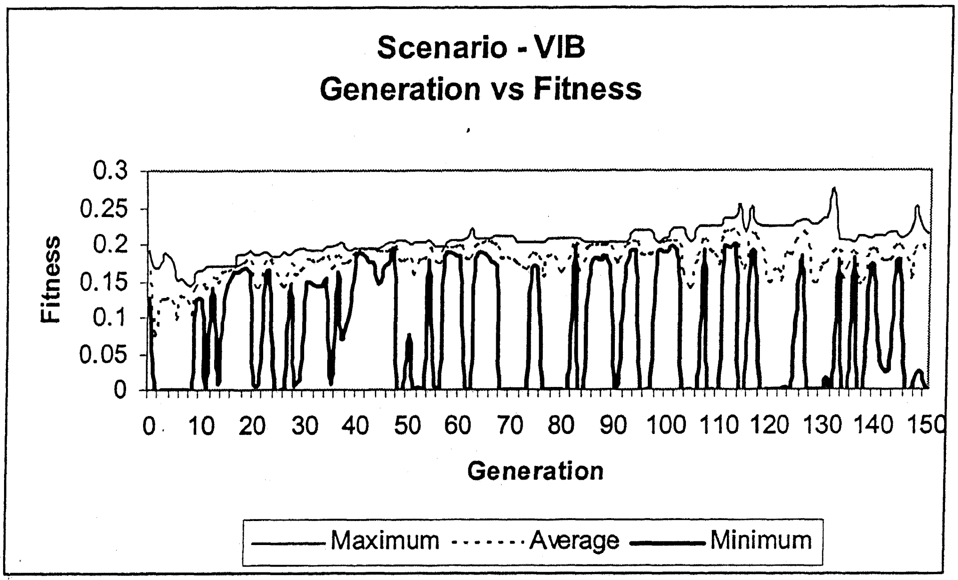


Figure 3.14 Generation vs. Fitness (Scenario-VIB).

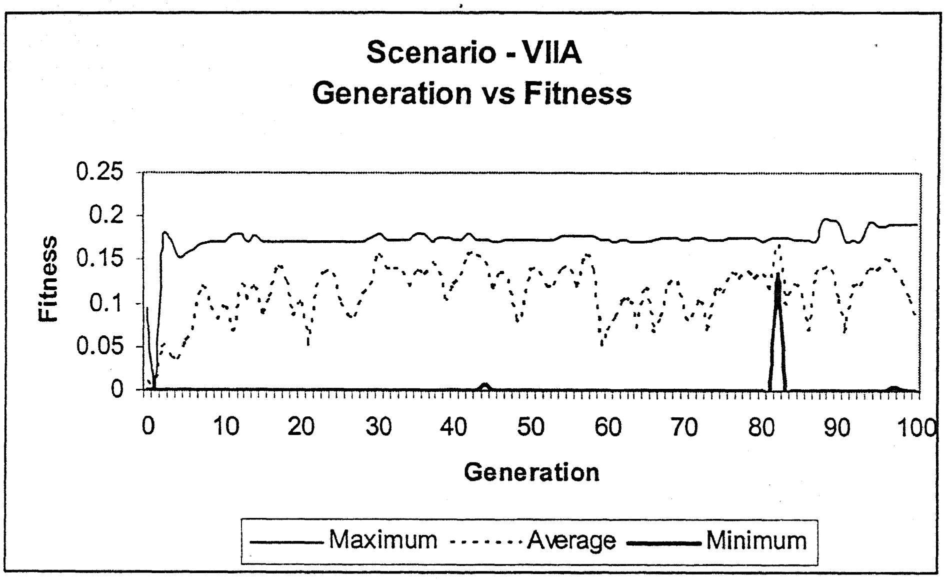


Figure 3.15 Generation vs. Fitness (Scenario-VIIA).

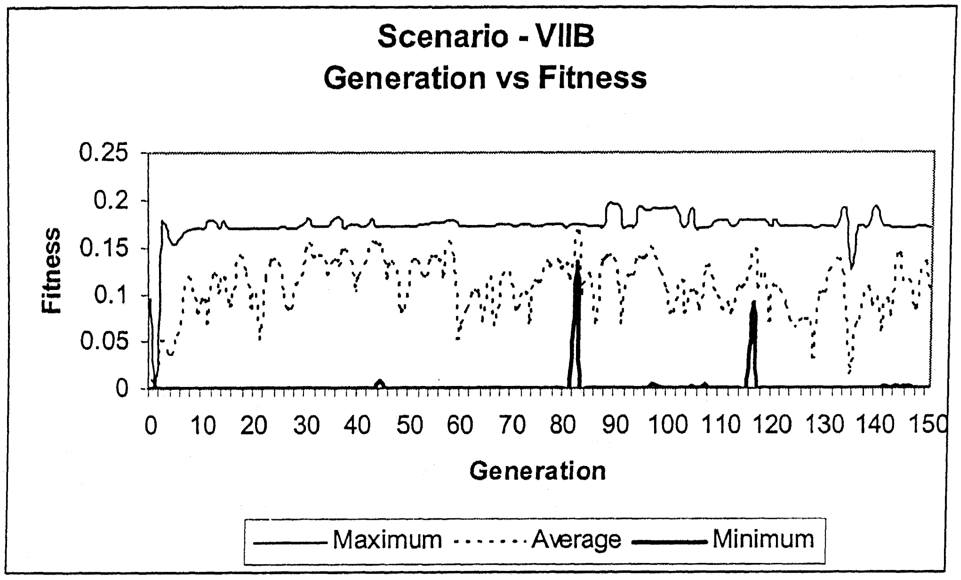


Figure 3.16 Generation vs. Fitness (Scenario-VIIB).

The solution results in terms of optimal pumping values for each of the scenarios I to VII, for two different numbers of permissible generations are shown in figures 3.17 to 3.30. These figures show the cumulative pumping rates over a total of three years pumping period at each of the five specified potential pumping locations.

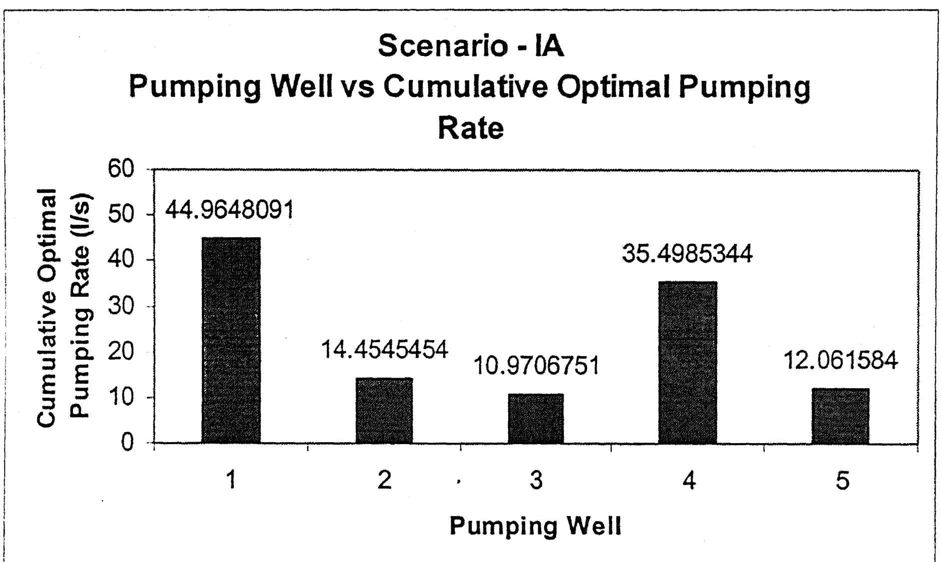


Figure 3.17 Cumulative optimal pumping rates (Scenario-IA).

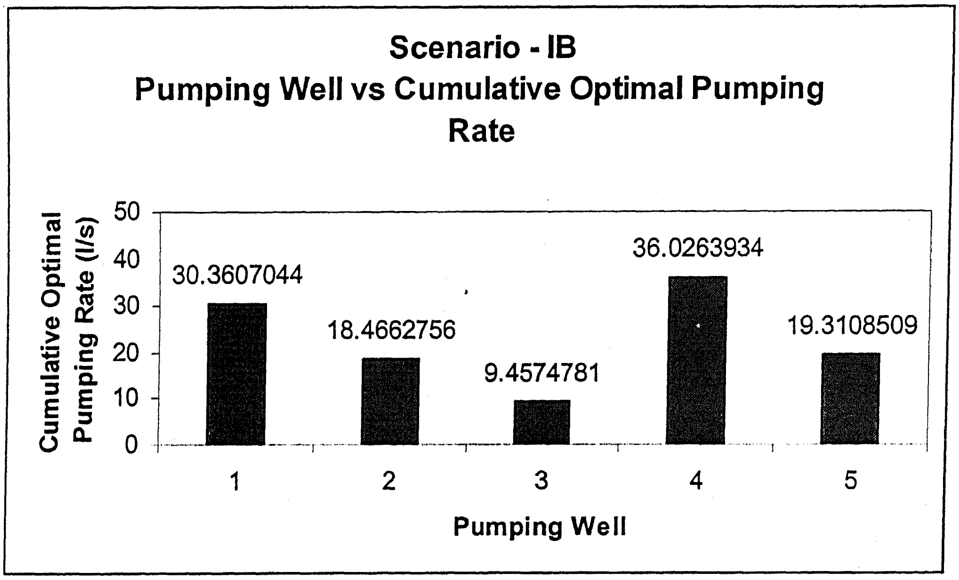


Figure 3.18 Cumulative optimal pumping rates (Scenario-IB).

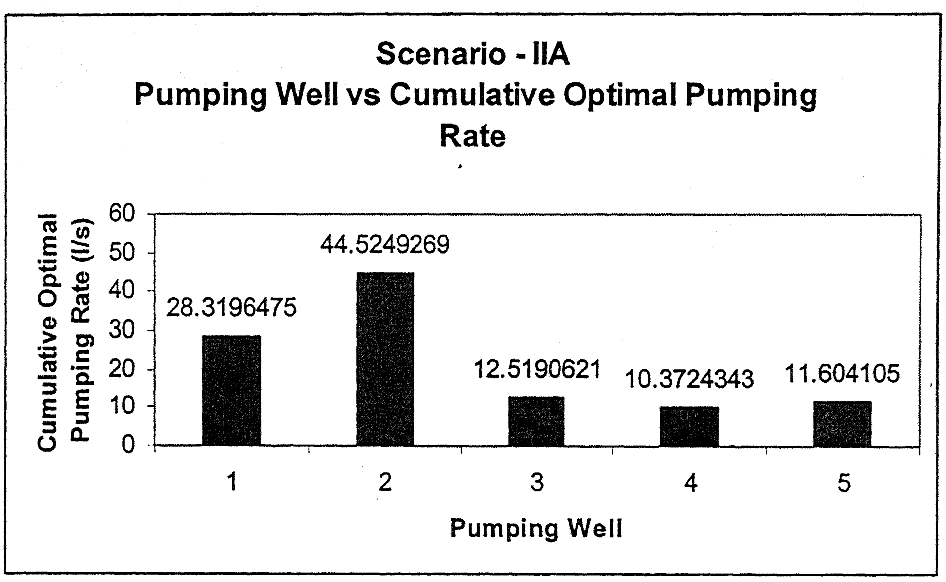


Figure 3.19 Cumulative optimal pumping rates (Scenario-IIA).

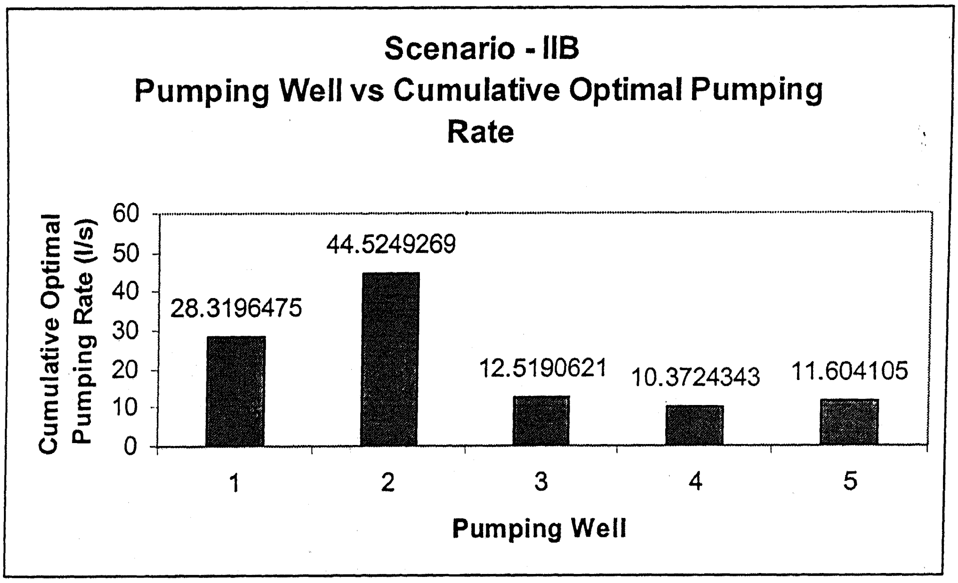


Figure 3.20 Cumulative optimal pumping rates (Scenario-IIB).

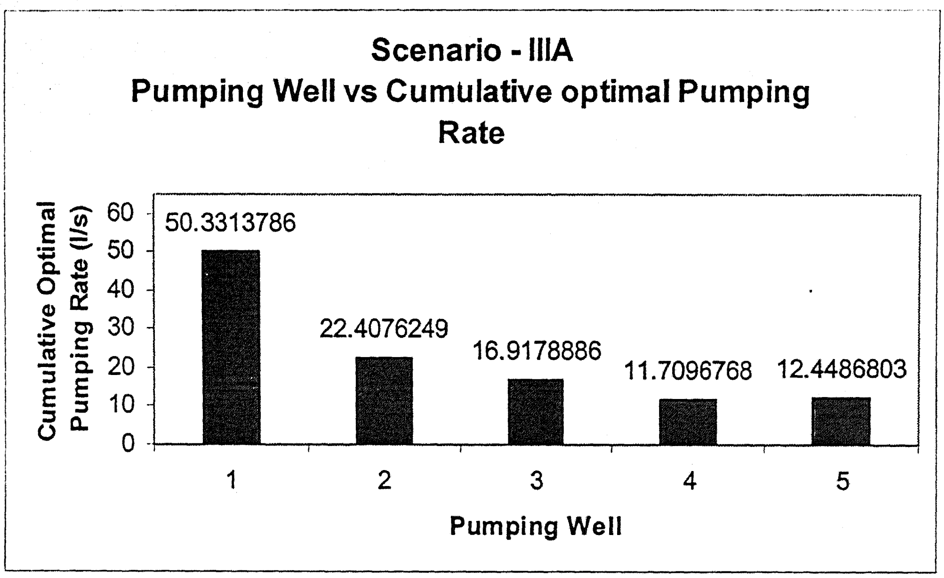


Figure 3.21 Cumulative optimal pumping rates (Scenario-IIIA).

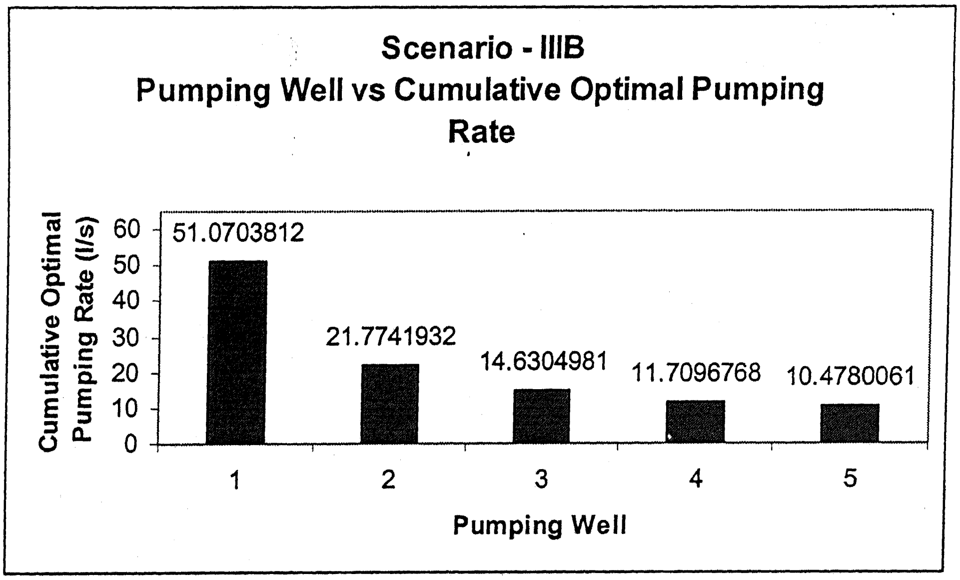


Figure 3.22 Cumulative optimal pumping rates (Scenario-IIIB).

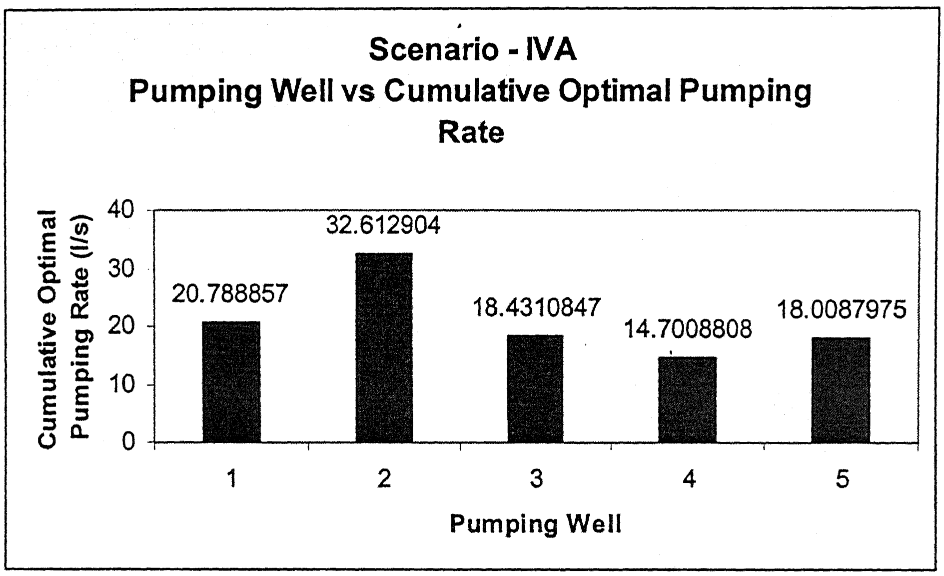


Figure 3.23 Cumulative optimal pumping rates (Scenario-IVA).

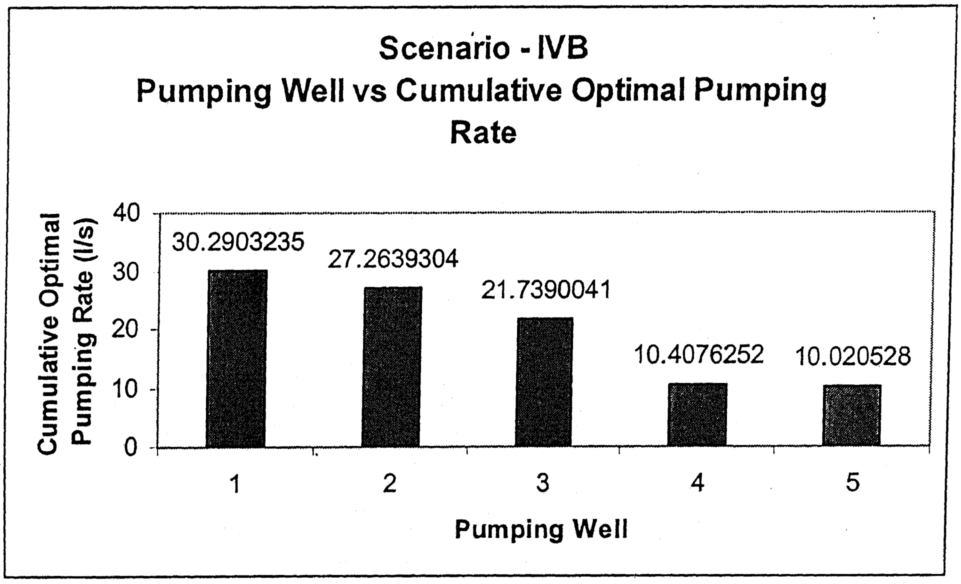


Figure 3.24 Cumulative optimal pumping rates (Scenario-IVB).

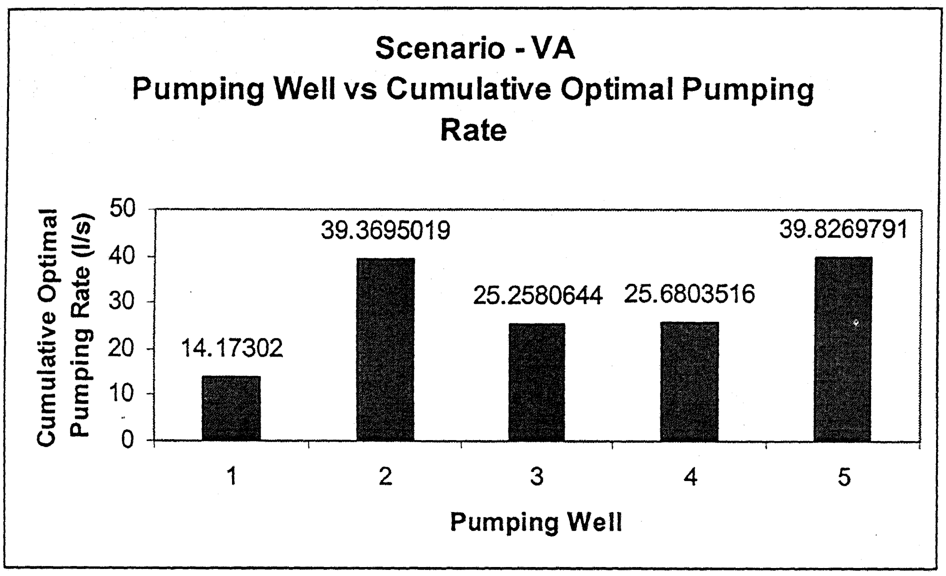


Figure 3.25 Cumulative optimal pumping rates (Scenario-VA).

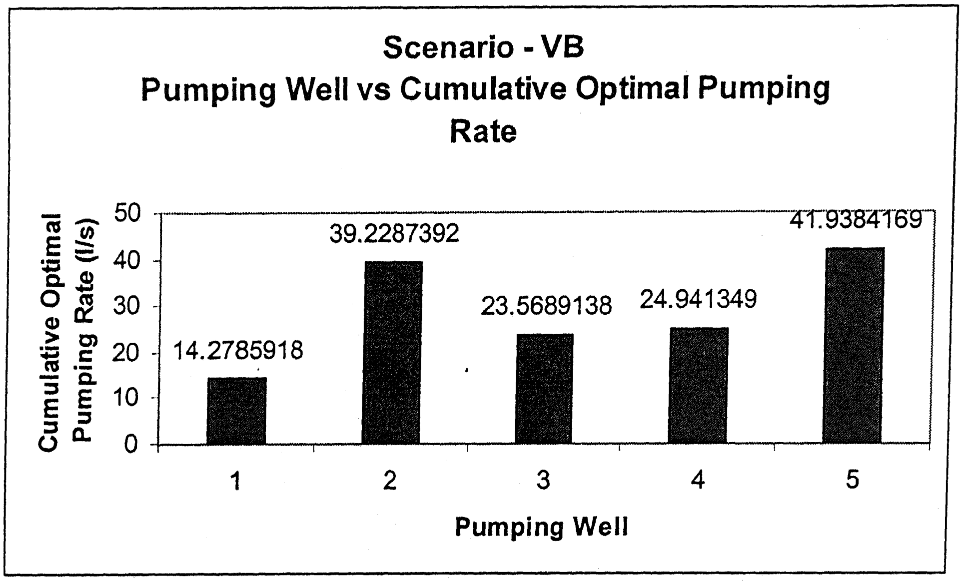


Figure 3.26 Cumulative optimal pumping rates (Scenario-VB).

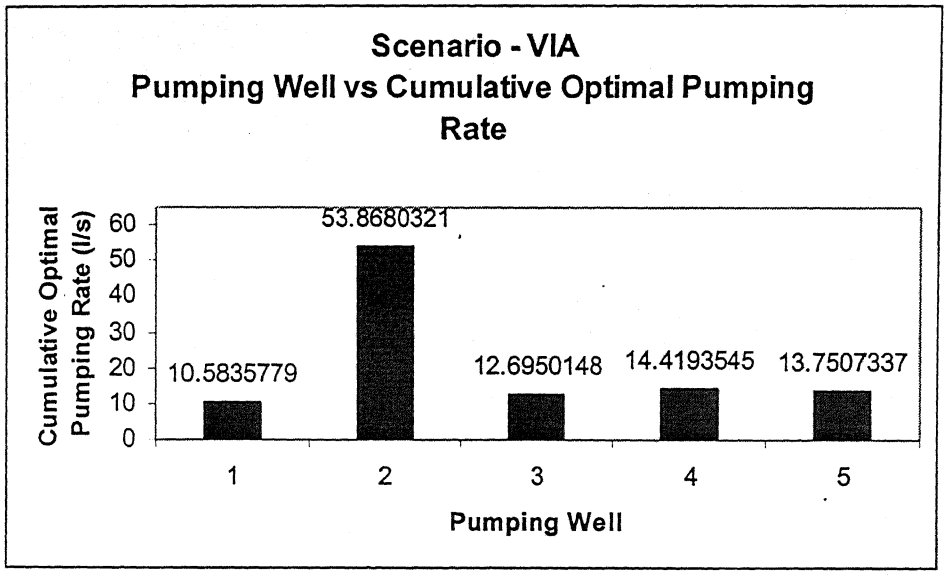


Figure 3.27 Cumulative optimal pumping rates (Scenario-VIA).

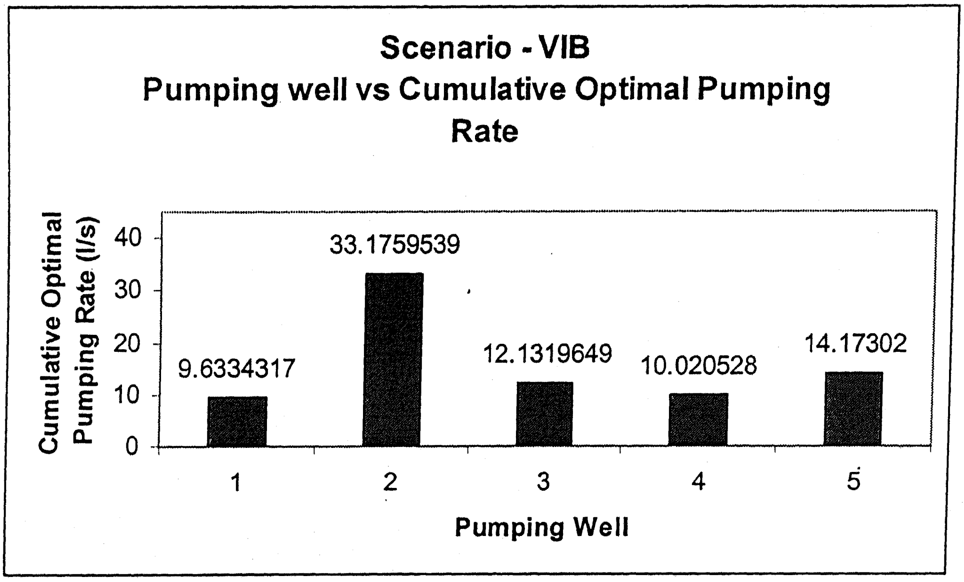


Figure 3.28 Cumulative optimal pumping rates (Scenario-VIB).

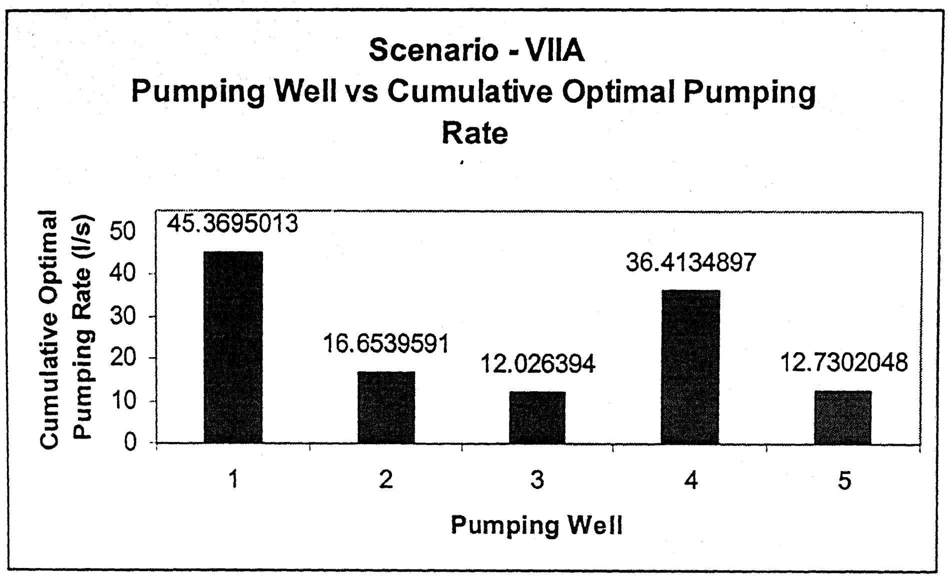


Figure 3.29 Cumulative optimal pumping rates (Scenario-VIIA).

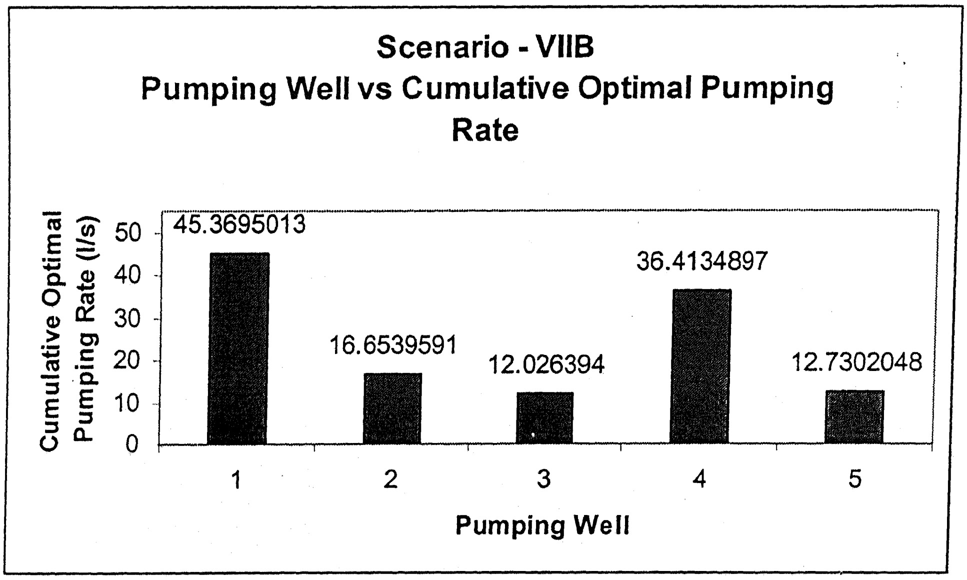


Figure 3.30 Cumulative optimal pumping rates (Scenario-VIIB).

3.7 Discussion of Results

The solution results obtained from the above mentioned scenarios are evaluated and discussed here. Different parameters that are changed in the above scenarios are: the maximum permissible number of generation in GA as specified, the maximum permissible concentration (C*) of the solute, upper limit of pumping rate at a given location and change of the location of the potential pumping wells.

The cumulative optimal pumping rates summed over all pumping locations and all management periods as obtained from the developed methodology are shown for each scenario in table 3.7. These pumping rates are also shown in figure 3.3.

Table 3.7 Cumulative optimal pumping rates.

Scenario	Cumulative Optimal Pumping Rate l/s
I-A	117.9501
I-B	113.6217
II-A	107.3401
II-B	107.3401
III-A	113.8152
III-B	109.6627
IV-A	104.5425
IV-B	99.7214
V-A	144.3079
V-B	143.9560
VI-A	105.3167
VI-B	79.1349
VII-A	123.1935
VII-B	123.1935

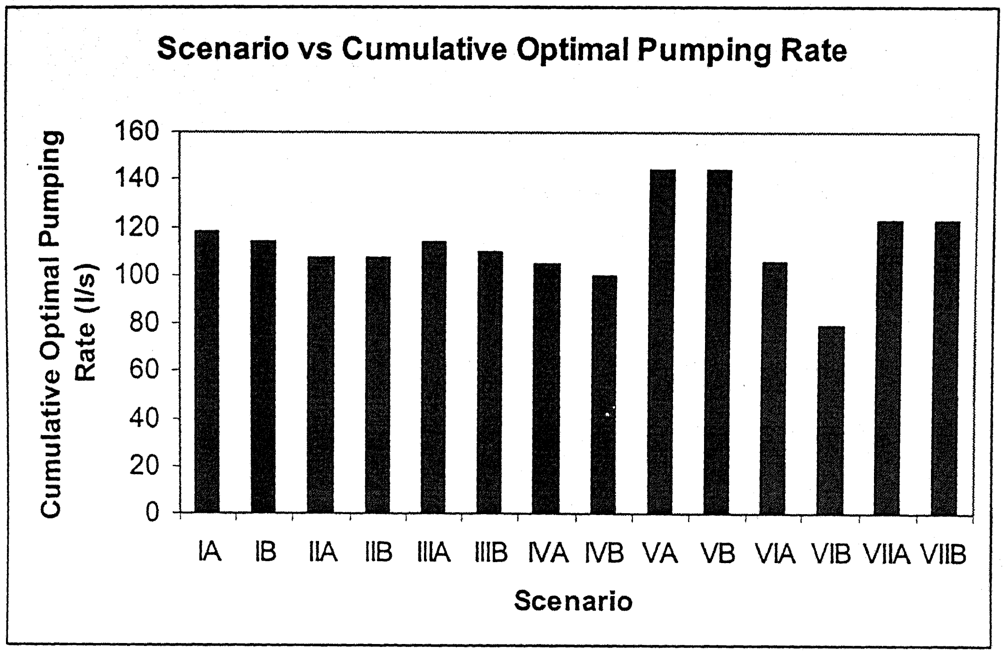


Figure 3.31. Cumulative optimal pumping rates.

3.7.1 Effect of Maximum Permissible Number of Generations

In all except two scenarios the solution obtained improved with increase in the maximum permissible number of generations in the GA, as specified. These results are as expected. However in scenarios II and VII this improvement is not evident. This may be due to the fact that the obtained solution did not improve with just fifty more generations for a population size of ten.

The plots of average, minimum and maximum values of the fitness function at every generation vs the numbers of generations (figures 3.3 to 3.16) show that the average fitness in general is not converging to the maximum fitness value as expected, when an optimal solution is near. However, the maximum fitness values do tend to stabilize or maintain a given level after about 60 to 80 generations in few cases. Therefore, in order to save computation time especially, when repeated solutions are necessary for evaluation purpose, the numbers of generations were limited to 100 or 150 only. A typical solution for 100 generations took about 3 hours of computer time on the Linux cluster.

3.7.2 Effect of Change in Maximum Permissible Limit of Solute Concentration (C^*)

The maximum permissible limits of solute concentration (C^*) considered in this study are 10 mg/l and 5 mg/l. As the objective function is subjected to the concentration constraint, intuitively we can say that the relaxation in the constraints may improve the objective function value and vice-versa. By comparing the solutions of scenarios II, III, IV, V, VI, and VII from table 3.7 we can observe that the objective function value, i.e., the cumulative optimal pumping rate required over space and time is larger when C^* is 5

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mg/l than when C^* is 10 mg/l. The cumulative optimal pumping rates are more in the scenarios III, V, VII, in which C^* is taken as 5mg/l compared to those for scenarios II, IV, VI in which C^* is taken as 10mg/l. This shows that more pumping is required to satisfy lower limits on maximum permissible concentration of the solute in the aquifer. This is expected, as lowering the permissible concentration limits actually reduces the feasible space. Therefore, the objective function value (minimization) increases. In these comparisons, the upper limit on pumping and the location of the pumping wells are identical for all the scenarios compared. In general, the same trend is evident when the number of generations is 100 or 150.

3.7.3 Effect of Change in the Upper Limit of Pumping

The upper limits on pumping adopted in this study are 15 l/s and 21 l/s. The upper limit of pumping is changed only in the wells P_1 and P_2, which are located upstream of the injection wells in all the scenarios. As more pumping is done on the upstream side, when the pumping limit is increased, the cumulative pumping required decreases and the spread of the contaminant plume is controlled. This is verified by comparing the solutions of the scenarios I, IV, V in which the upper limit on pumping is 15 l/s with those for scenarios II, VI, VII, in which the upper limit on pumping is 21 l/s for the pumping wells P_1 and P_2. In these comparisons, the maximum permissible limit of solute concentration and the location of the pumping wells are identical for the scenarios compared. A discrepancy is observed in the solutions obtained for scenarios IVA and VIA. These counter intuitive results may be due to the fact that the obtained solutions for 100 generations may be far away from the actual optimal solutions.

Table 3.8 Objective function values as a function of number of generations.

Generation number	Objective function value
214	96.4488
311	94.689
584	91.8387
639	90.1497
641	88.5309
642	88.4955
693	85.8915
838	85.8564
839	83.604
862	83.3577

In order to verify this, numerical experiments were conducted by increasing the maximum number of generations to 1500. From the results of these experiments it is evident that the maximum number of generations specified is very important for obtaining optimal solutions. As shown in table 3.8, it is also observed that there is substantial improvement in the objective function value by increasing the maximum number of generations from 150 to 1500. As shown in table 3.8 the fitness values increases substantially as the number of generations increase. These solutions results for 1500 generations tend to justify the discrepancies observed while comparing the solutions results for scenarios e.g. IVA and VIA. These discrepancies may not occur if all the comparisons are based on actual optimal solutions.

3.7.4 Effect of Change of the Pumping Location

To study the effect of change in the pumping location, location of two wells P_2 and P_3 are changed from (9,9) and (11,4) to (10,9) and (10,5) respectively in the above scenarios. The well locations are shifted nearer to the injection wells I_1 (8,5) and I_2 (12,9). It is possible that by locating the pumping wells nearer to the injection wells the transport

of the contaminant can be controlled more effectively. This is verified by comparing the obtained solutions. By comparing the solutions for scenarios I and II with those for scenarios IV and VI, it is seen that by introducing pumping wells closer to the pollutant injection location, the optimal solution for optimal strategy can be improved further. The change in location of the pumping wells results in more efficient solutions. Therefore, cumulative pumping rates for scenarios IV and VI are better than those for scenarios I and II respectively, as shown in table 3.7 and figure 3.31. The effect of change in the pumping locations on the individual pumping rates, are evident from figures 3.17 to 3.30. the pumping rates at wells P2 and P3 with changed locations is greater than those before shifting the locations. However, the total pumping from all the wells is lesser. There is a discrepancy in the comparison of solution for scenarios III and VII. The possible reason for these discrepancies may be the inadequacy in the number of generations permissible, as discussed earlier. The conclusions of this study are presented in the next chapter.

Chapter 4

Summary and Conclusions

4.1 Summary

A methodology was developed for optimal management of a contaminated aquifer, incorporating biodegradation. The aim was to obtain optimal pumping strategies in a contaminated aquifer, in order to limit the spatial and temporal concentrations within specified permissible limits. A hydrocarbon Toluene was assumed to be pollutant, which also undergoes biodegradation in the aquifer.

A linked simulation optimization model was developed and solved using a binary coded Genetic Algorithm (GA) externally linked to a numerical model for the simulation of flow and transport in an aquifer with advection, dispersion, and biodegradation. The constrained linked simulation-optimization model was converted to an unconstrained optimization problem using the exterior penalty function approach.

The performance of the developed methodology was evaluated for a specified study area with different management scenarios.

4.2 Conclusions

1. The performance evaluation results show that the developed methodology is potentially applicable for obtaining optimal pumping strategies in a contaminated aquifer, incorporating biodegradation process.
2. The solution results in general match with intuitive results, with few discrepancies noted.

3. The pumping required increases with decrease in the permissible limit on pollutant concentrations.
4. The potential pumping locations have significant effect on the total pumping rate required to control the pollutant concentration.
5. The number of generations used as a termination criterion for the GA, is very important in ensuring the optimality of the solution obtained.
6. Few solution results which when compared were counter intuitive. This may be due to the local and not global optimality of the solutions.
7. Increase in the permissible upper limit of pumping rates may be actually decrease the total pumping required, as it allows more pumping at more efficient pumping locations.

4.3 Scope for Future Work

1. The real coded GA may be more efficient in solving the optimization problem and may be utilized.
2. Introduction of elitism could improve the efficiency of the GA and therefore elitist GA with different stopping criteria needs to be tested.
3. The applicability of this methodology while incorporating multiple species and additional transport processes may be tested.
4. This methodology needs to be evaluated for a larger study area with real life data, to establish its applicability in real life situations.

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